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Guideline for Use of City-Specific EKMA in Preparing Ozone SIPs

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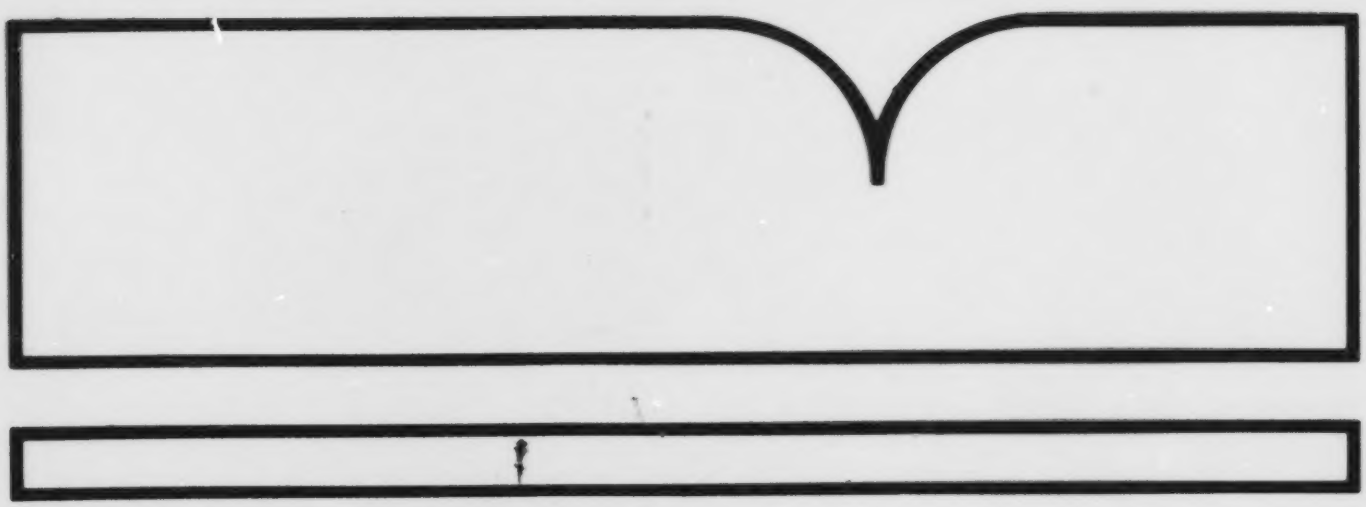

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Report describes how to use the city-specific EKMA model as a means for estimating emission control requirements needed to demonstrate attainment of the ozone NAAQS in 1982 SIP's. Topics addressed include (a) use of air quality, meteorological and emissions measurements or estimates for generating ozone isopleth diagrams; (b) application of the ozone isopleth diagrams in estimating controls needed to attain the ozone NAAQS at each monitoring site; and (c) estimation of the city-wide control requirement for use in the SIP.

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Guideline For Use Of City-specific EKMA In Preparing Ozone SIPs

Air Management Technology Branch
Monitoring and Data Analysis Division

U.S. ENVIRONMENTAL PROTECTION AGENCY
Office Of Air, Noise, and Radiation
Office of Air Quality Planning and Standards
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SUMMARY

This summary outlines the procedure used in applying city-specific EKMA in State Implementation Plans (SIPs) for ozone. City-specific EKMA consists of two components: the OZIPP model and the EKMA procedure (i.e., OZIPP/EKMA).

OZIPP (Ozone Isopleth Plotting Package) is a computer program which allows the user to plot maximum hourly ozone concentrations as an explicit function of initial (e.g., 8 a.m.) ambient concentrations of the precursors non-methane organic compounds (NMOC) and oxides of nitrogen (NO_x). The resulting output is an ozone isopleth diagram. Because the OZIPP model allows consideration of meteorological inputs, pollutants transported from upwind and precursor emissions which are appropriate for each city under review, the isopleths are also implicit functions of these variables.

EKMA (Empirical Kinetic Modeling Approach) is a procedure for applying the ozone isopleth diagram obtained with OZIPP to estimate the impact of controlling urban volatile organic compound (VOC) and/or NO_x emissions on peak hourly ozone concentrations. Ambient 6-9 a.m. NMOC/NO_x ratios measured in the urban core and peak hourly ozone measured within or downwind of the city are needed to apply an isopleth diagram in the EKMA procedure.

Because urban VOC and/or NO_x emission reductions are likely to be more effective under some conditions than others, there is not necessarily a simple 1:1 correspondence between high observed ozone concentrations and emission controls estimated as necessary to attain the National Ambient Air Quality Standard (NAAQS) for ozone. Thus, in order to ensure that the standard is attained, it is necessary to perform city-specific EKMA modeling for several days. This provides more

complete assurance that the standard will be met if a control target is achieved. Consideration of the five days with the highest observed daily maximum ozone concentrations at each site affected by the urban area is believed to be sufficient.

The procedure for applying city-specific EKMA is outlined in the following seven steps. Each step is discussed in greater depth in the indicated section(s) of this report.

1. Select the five days with highest maximum hourly ozone concentrations observed at each site affected by the urban area over the past three years (Section 2.1).

2. For each of these days, estimate the 6-9 a.m. NMOC/NO_x ratio prevailing in the urban core (Section 3.2.2).

3. Using the input data summarized in Table S1, apply the OZIPP computer program to generate ozone isopleth diagrams for each day. The exact procedure is described in User's Manual for Kinetics Model and Ozone Isopleth Plotting Package, EPA-600/8-78-014a. The resulting diagrams denote sensitivity of peak hourly ozone concentrations to locally generated precursors, given a set of "current" accompanying conditions (e.g., a specified concentration of transported ozone from upwind sources).

4. Using the ozone concentrations obtained in Step 1 and the NMOC/NO_x ratios derived in Step 2, establish a "starting point" on each of the ozone isopleth diagrams obtained in Step 3 (Section 4.1).

5. If there is a change(s) in the base case conditions assumed to prevail in generating isopleth diagrams obtained in Step 3, it is necessary to

Table S1. Inputs Needed to Generate an Ozone Isopleth Diagram

Input	How Used and Obtained	Section(s) of Report Describing Process in Detail
(1) Light Intensity	Enter the date and a city's latitude, longitude and time zone to the OZIPP program.	Section 3.1.1
(2) Atmospheric Dilution	Use National Weather Service (NWS) or Urban Radiosonde data and urban surface temperatures to estimate 8 a.m. mixing height, maximum daily mixing height and the time which the maximum daily mixing height occurs. In the event NWS or urban data are unavailable, use values compiled in Table A-1.	Section 3.1.2 Appendix A
(3) Present Transport of Ozone	The model assumes that ozone is transported in two layers: at the surface and aloft. Ozone transported at the earth's surface is generally assumed to be zero. Ozone transported aloft can be estimated using mid-morning ozone concentrations observed at a continuously operated surface monitor located upwind of the city on each day considered.	Section 3.1.3
(4) Present Transport of Precursors	Measurements and past model applications have indicated the impact of transported precursors is generally negligible. Hence, these are ordinarily assumed to be zero. In cases where there is reason to believe precursor transport is high, special procedures are needed. These procedures require 6-9 a.m. measurements of precursor concentrations upwind of the city obtained by summation of organic species.	Section 3.1.4 Appendix B
(5) Post 8 a.m. Emissions	Derived using 6-9 a.m. ambient NMOC and NO_x measurements in the urban core on each day modeled, seasonal countywide VOC and NO_x emission inventories and information concerning the location of the maximum observed ozone concentration on each day modeled.	Section 3.1.5
(6) Reactivity	Recommended default values should be used.	Section 3.1.6

generate a second set of isopleth diagrams. This second set of diagrams reflects the impact of changing the set of "current" accompanying conditions described in Step 3. For example, a second set of diagrams is most frequently used to allow the user to consider changes in ozone transported into a city. In such an application, the second set of diagrams is obtained using an assumed future concentration of transported ozone. Suggested procedures for estimating future transported ozone are described in Section 4.2.1.

6. VOC and/or NO_x controls needed to reach 0.12 ppm O_3 on each day at each site are estimated using the starting point on each diagram representing the current conditions (Step 4) and calculating controls needed to reach the 0.12 ppm ozone isopleth on the corresponding diagram obtained in Step 5. This procedure enables the user to consider concurrent changes in local precursor emissions and in such variables as transported ozone from upwind sources.

7. As a result of Step 6, there is one estimate of VOC controls needed to reach a peak hourly ozone value of 0.12 ppm at each site for each day. Each of these estimates is valid only for the best estimate of changes in NO_x between the base year* and 1987. The site specific VOC emission reduction is the fourth highest control estimate, assuming a three-year data base. If there were only one year of data at a site, the control requirement would be the second highest control estimate; two years of data, the third highest control estimate, etc. Because of possible significant changes in emissions or emission patterns over longer periods, a three-year sampling period is the maximum which should

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* Normally the base year is 1980.

normally be considered. The SIP VOC emission reduction for the urban area is the highest site-specific control estimate. Selection of the target control goal for a SIP is illustrated in Table 2.2.

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1.0 INTRODUCTION

This document is intended to fulfill several purposes:

1) to describe application of a relatively simple modeling procedure, city-specific EKMA, which is useful for estimating the effectiveness of reducing emissions of volatile organic compounds (VOC) and/or oxides of nitrogen (NO_x) in reducing peak ozone values downwind or within a city;

2) to indicate how available emissions, air quality and meteorological data are used in the modeling procedure;

3) to provide one means for Air Pollution Control Agencies to check the completeness and suitability of analyses performed with the model to support the need for urban VOC and/or NO_x emission controls.

The city-specific EKMA modeling procedure has also been referred to as "Level III analysis." These terms are synonymous. City-specific EKMA consists of two components: the OZIPP model and the EKMA procedure (i.e., OZIPP/EKMA).[1,2,3] "OZIPP" (Ozone Isopleth Plotting Package) is a computer program which allows the user to plot maximum hourly ozone concentrations as an explicit function of initial (8 a.m.) ambient concentrations of non-methane organic compounds (NMOC) and NO_x within the urban area.[4] The resulting output is an ozone isopleth diagram. Although the ozone isopleths are explicitly plotted as a function of initial NMOC and NO_x, they are also implicit functions of numerous other variables. For example, the role of subsequent VOC and NO_x emissions, meteorology and pollutants transported from areas upwind of the modeled city are also considered in OZIPP.

"EKMA" (Empirical Kinetic Modeling Approach) is a procedure for applying the ozone isopleth diagram generated with the OZIPP to estimate the impact of changing urban VOC and/or NO_x emissions on peak hourly ozone concentrations. Two pieces of information must be available to apply EKMA: the 6-9 a.m. ambient NMOC/NO_x ratio prevailing in the urban area, and the peak hourly ozone concentration measured within or downwind of the city. These two pieces of information provide a starting point on the isopleth diagram from which to estimate control requirements.

The conceptual basis for the isopleth diagram is a Lagrangian model (OZIPP) which follows the evolution of ozone from precursors within a migrating column of air. The column of air extends from the earth's surface throughout the mixed layer. All pollutants are uniformly mixed within the column. From early morning to mid-afternoon, the height of the column increases due to the diurnal rise in mixing height. This results in simultaneous dilution of pollutants within the column and entrainment of additional pollutants from above the mixed layer. Concurrently with the foregoing dilution and entrainment, fresh precursor emissions encountered as the column is transported by the wind are injected into it. All resulting pollutants within the column of air are assumed to react chemically in accordance with the chemical kinetic mechanism in OZIPP.

The data base needed to develop isopleth diagrams in accordance with the model formulation described in the previous paragraph is summarized in Table 1-1. Such a data base is consistent with what has been described on pages 65669-65670 in the November 14, 1979, Federal Register as a "Level III" analysis.[5] The data are adequate for insuring that the observed peak ozone value has, indeed, occurred within or downwind of the city being reviewed. However, the data are not adequate for tracing the exact trajectory leading to the peak ozone value, nor for precisely

Table 1-1. Data Requirements for Use of City-Specific EKMA

Data Item	Requirements
1. Air Quality Data	
A. Ozone Monitors	- Minimum of 3 sites; one upwind the second on downwind edge of city and the third 15-40 km downwind. (See EPA-450/2-77-021a and Section 3.1.3)
B. Precursor Data	- Minimum of 1 site with collocated NMOC and NO_x monitors, with two sites desirable. (See EPA-450/4-80-011 and Section 3.2.2)
2. Meteorological Data	
A. Upper Air Data	- National Weather Service Rawinsonde data if available. (See Section 3.1.2 and Appendix A)
B. Surface Temperature and Pressure Data	- Hourly surface temperature and pressure data at one site in the urban area. (See Section 3.1.2)
C. Surface Wind Data	-Minimum of two sites; one in high precursor area and one additional site. (See Section 3.2.1)
3. Emission Data	
A. VOC Emissions	- A seasonally adjusted, countywide, annual emission rate for each broad source category. (See Section 3.1.5)
B. NO_x Emissions	- A seasonally adjusted, countywide, annual emission rate for each broad source category. (See Section 3.1.5)

estimating emissions injected into a particular column of air. The procedures described in this document therefore make assumptions about the trajectory of the modeled column of air. The column is assumed to be within the urban area at 8 a.m. and to migrate downwind in a straight line to the site observing the peak ozone concentration by the time the peak is observed.* Although use of city-specific input data should improve model accuracy, the limited data base and the resulting assumptions made in applying the city-specific EKMA (i.e., Level III analysis) still make it uncertain that the model will always perform well in an absolute sense. That is, one would not necessarily expect to be able to measure NMOC and NO_x downtown and then use the isopleth diagram to predict peak ozone concentrations. However, sensitivity studies have shown that differences resulting from incomplete input data or gross assumptions employed by the model tend to exhibit proportional impacts on the positions of various ozone isopleths on an isopleth diagram.[10] Thus, the model should perform satisfactorily when applied in a relative sense (e.g., to estimate a change in peak ozone accompanying changes in local precursor levels).

City-specific EKMA is expected to be widely used in preparing State Implementation Plans (SIPs) submitted to attain the National Ambient Air Quality Standard (NAAQS) for ozone. The NAAQS for ozone is now in a statistical form (i.e., daily maximum ozone concentrations are <u>not expected</u> to exceed 0.12 ppm more than once per year). Because urban VOC and/or NO_x emission reductions are

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* Because a review of St. Louis RAPS data has suggested that ordinarily the diurnal variation in urban NMOC/NO_x ratio is small, it is not regarded as critical that the column of air be within the urban area at precisely 8 a.m. It should be sufficient if the air is within the urban area by mid-morning. If extensive wind data suggest that the column of air is still upwind of the urban area at noon or later, problems of this nature need to be addressed on a case by case basis in consultation with the EPA.

likely to be more effective under some conditions than others, there is not necessarily a simple 1:1 correspondence between high observed ozone concentrations and estimated emission controls needed to attain the ozone NAAQS. Thus, in order to ensure that daily maximum ozone concentrations are not expected to exceed 0.12 ppm more than once per year, it is necessary to apply city-specific EKMA to several different days observing high ozone concentrations. This differs from common past practices in which a single ozone design value was selected and control requirements were calculated based solely on this value. Chapter 2.0 describes the procedure, underlying rationale, and key issues which arise in applying city-specific EKMA on several days.

Data needs for applying city-specific EKMA on each day selected pursuant to guidance in Chapter 2.0 have been summarized in Table 1-1. Chapter 3.0 discusses how these data are transformed into input to city-specific EKMA. The discussion concerning each input variable follows a consistent format. First, it is assumed that valid data have been collected as specified in the Federal Register. The most appropriate procedure for transforming these data into each input variable is identified. However, it is also recognized that the available data will not always conform exactly to the Federal Register specifications. For example, in a few cases, the data base may be more detailed than what is specified in the Federal Register. Procedures are described for utilizing such a data base if so desired. More often, some data may be missing or subsequently determined to be invalid. Procedures for deriving model inputs under such circumstances are also identified. In the event that quality assured NMOC and NO_x data cannot be obtained for a sufficient number of days to provide a reliable estimate of the prevailing NMOC/NO_x ratio, city-specific EKMA cannot be used.

Once all of the input has been prepared consistently with guidance in Chapter 3.0, the OZIPP model is used to generate ozone isopleths for each of the days identified as necessary. The EKMA procedure is then applied to each set of isopleths to estimate the amount of VOC and/or NO_x controls needed to reduce the peak hourly ozone concentration to 0.12 ppm on each day. From these estimates, the amount of VOC and/or NO_x control is selected such that a peak hourly O_3 concentration of 0.12 ppm will not be expected to be exceeded on more than one day per year. Chapter 4.0 illustrates the application of city-specific EKMA to estimate controls for each day. The determination of the SIP control requirement is described in Section 2.3.

2.0 ESTIMATING CONTROL REQUIREMENTS FOR 1982 OZONE SIPs

Prior to discussing procedures for estimating control requirements with city-specific EKMA, it is appropriate to address the National Ambient Air Quality Standard (NAAQS) for ozone. The NAAQS affects the choice of ozone values input to EKMA, as well as the stringency of a city's calculated control requirements.

The National Ambient Air Quality Standard for ozone is attained when the expected number of days per calendar year, with maximum hourly average concentrations above 0.12 ppm, is less than or equal to one.[6] This differs from the previous photochemical oxidant standard which specified a concentration "not to be exceeded more than once per year."[7] As with the previous standard, air quality data are examined on a site by site basis and each site must meet the standard. The Guideline for the Interpretation of Ozone Air Quality Standards recommends that a period of three successive years of air quality data be used as the basis for determining attainment of the standard.[8] As more years of data are included, a greater chance exists for minimizing the effects of an extreme year caused by unusual meteorology. However, extending the number of successive years too far increases the risk of averaging data during a period in which a real shift in emissions and air quality has occurred.

Two important differences with past practices occur as a result of the new standard. First, only one hourly value is considered for each site on each day. This can affect the set of candidate "ozone design values" used to estimate the amount of controls needed to reach 0.12 ppm ozone. Formerly, extremely rare episode days with a number of very high ozone values at any given site were weighted disproportionately. The new standard inherently recognizes this problem by allowing only one concentration (and therefore one control estimate) to be

considered per site per day.

Second, the phrase, "... expected number of days per calendar year..." alleviates a concern with the former standard that those States which have maintained conscientious monitoring programs over the years are penalized. Since the expected or "average" number of days per year with daily maximum ozone concentrations greater than 0.12 ppm is of concern, this means that there can be more than one day observing ozone concentrations in excess of 0.12 ppm if the data base is two or more ozone seasons in length.

Another implication of the NAAQS is that the frequency distribution of ozone concentrations at each monitoring site which occurs after the implementation of controls is the key consideration in demonstrating attainment. This has always been the case. In the past, however, very simplistic models (e.g., rollback, envelope curves) were used to demonstrate attainment. Minimal use was made of meteorological or air quality data. Under such circumstances, choosing the ozone value to input into a model in order to calculate control requirements was very straightforward. The design value was simply the second highest value observed. The degree of control needed to attain the NAAQS, however, is a function of many things in addition to observed ozone concentrations during the base period. For example, controls needed to attain the NAAQS are a function of pollution transported from upwind sources, prevailing NMOC/NO_x ratios and atmospheric dilution. Therefore, it is conceivable that the second highest ozone design value would not require the second highest control requirement to attain the NAAQS if one uses city-specific EKMA or more sophisticated models. Of paramount interest is the frequency distribution of control estimates calculated with such models. Depending on the length of the period of record at any given monitoring station, one

would choose the control estimates which would insure that, on average, the daily maximum hourly ozone concentration would not exceed 0.12 ppm more than once per year at any monitoring site. For example, if the period of record at one site were three years, the fourth highest calculated control estimate would be chosen as demonstrating attainment at that site. The control requirement needed to demonstrate attainment for the city as a whole is whatever is necessary to demonstrate attainment at all ozone monitoring sites. Therefore, it is necessary to model a number of high ozone days to determine the degree of control required to attain the ozone standard.[1] This need, while always present, can now be adequately addressed due to increased data availability. Given this situation, demonstration of attainment could entail generating isopleths for (1) each site and each day above 0.12 ppm ozone, or (2) for each set of meteorological conditions, with associated probabilities of occurrence, that may result in violations of the NAAQS. Depending on the nature of the ozone problem for a given city, either approach would require generating several isopleth diagrams. Because it is relatively easy to generate these diagrams and apply EKMA, procedures described in the next Section recommend examining several days and monitoring sites without very elaborate procedures to eliminate a number of candidate days prior to the modeling. Persons using more sophisticated modeling procedures would most likely find it preferable to develop screening procedures to eliminate a number of candidate days prior to the modeling exercise.

Even for city-specific EKMA, given the size of monitoring networks and the expected number of observed ozone concentrations greater than 0.12 ppm in many urban areas, the computer costs and manpower requirements for the two approaches mentioned above might exceed the resources available to many State and local

agencies. Therefore, in developing a procedure for estimating urban area control requirements, consideration has been given to resource requirements, model complexity and model input requirements, as well as to the form of the ozone standard.

2.1 SELECTION OF DAYS TO MODEL

Control estimates obtained with city-specific EKMA can be sensitive to such factors as the level of ozone transported into an urban area.[2] Thus, control estimates based on the "classical design day" could understate the degree of control required for the city to attain the NAAQS. As a result, several days should be selected for modeling.

Recommended Procedure: For each ozone monitoring site, the five (5) days with the highest daily maximum ozone concentrations should be selected as candidates for modeling. In selecting the days for each site, only those days on which ozone values are observed downwind or within the urban area should be considered. Determination of what is "downwind" on a given day requires the review of prevailing wind data for that day. Such a review may, in fact, reveal that a nominally "downwind" site is in actuality upwind of the city on a particular day (see Figure 3-2 for an example of "upwind" versus downwind areas). If this is the case, the ozone value observed at that site should not be modeled. The days should be chosen from the most recent three (3) years for which measurements were made at the site. By limiting the number of days to model, this approach represents a compromise between a strict interpretation of the ozone standard and consideration of model complexity and local agency resources. However, the control estimates obtained with this procedure should not differ significantly from those obtained by modeling each site and day above the ozone standard. EKMA, when used in this manner, serves as a "screening procedure" for identifying the control strategy design day. With more sophisticated models, other (e.g., statistical) techniques may prove to be more viable for selecting days to model for control strategy evaluations.

Alternate Procedure: Alternative attainment demonstrations might include modeling each day in which the NAAQS was exceeded during the past three years, or modeling a statistically determined design day or set of meteorological classes. Probabilistic approaches, however, may be more difficult to develop and implement than simply using EKMA itself as the screening procedure.

2.2 DAY SPECIFIC CONTROL ESTIMATES

Once the days to be modeled are selected, control estimates must be calculated

for each of these days. Considerable duplication in high ozone days is likely for many of the sites in the monitoring network. When this occurs, the same isopleth diagram can usually be used to make control estimates for a number of sites.

Recommended Procedure: The OZIPP should be used to generate an isopleth diagram for each day identified as described in Section 2.1. Preparation of the model input data is described in Section 3.1. Development of a second isopleth diagram may be necessary if different control measures are implemented concurrently, e.g., reductions in future levels of ozone transported aloft. Procedures for handling this situation are presented in Chapter 4.

Two additional pieces of information are needed to calculate control estimates for each day and site: the daily maximum ozone value at each site and the urban 6-9 a.m. NMOC/NO_x ratio. Section 3.2.2 provides procedures for determining the appropriate ratio for use in city-specific EKMA.

Having assembled the necessary data and generated an ozone isopleth diagram for each selected day and (if necessary) each site,* the VOC reduction necessary to lower the peak ozone selected value to 0.12 ppm is calculated for each day at each appropriate site. The procedures for calculating control estimates using the isopleth diagrams are described in Chapter 4.

2.3 SIP CONTROL REQUIREMENT

The control requirement for use in the 1982 ozone SIPs is determined from the control requirements estimated for each site.

Recommended Procedure: Given the form of the ozone standard, the SIP control requirement is that control estimate with frequency of occurrence of 1/365 for the controlling site. Thus, having modeled the five highest days at each site, it is assumed that the upper portion of the control requirement distribution has been defined. Table 2-1 indicates which control estimate would be selected as the control requirement for each site. The SIP control requirement is the highest of the site-specific control requirements.

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* Often, it will not be necessary to generate as many diagrams as implied by this procedure. For example, if high ozone values occur at two or more sites on the same day, with rare exceptions, the same diagram can be used. One exception to this generalization is discussed in Section 3.1.5.

Table 2-1. Tabular Estimation of Site-Specific Control Requirements

Number of Complete Ozone Seasons Monitored*	Data Point Used for Site-Specific Control Requirements
1	Second highest control estimate
2	Third highest
3	Fourth highest

* Monitoring data at a site is considered to be complete if valid daily maximum hourly concentrations exist for at least 60 days during the ozone season. If a site does not meet this criterion during any of the last three ozone seasons, the second highest control estimate calculated at a site is the site-specific control requirement. In order for a season's daily maximum ozone values to be valid, there can be no systematic pattern of missing potential peak hours in the data base.

Table 2-2 contains an example of the procedure for selecting SIP control requirements for urban areas. In constructing this example, it is assumed that the urban area has three ozone monitoring sites: Site A within the city, Site B in the predominantly downwind direction from the city, and Site C in the predominantly upwind direction of the city. Site A has two (2) years of ozone data, Site B has three (3) years of data, and Site C has only one (1) year of ozone data.

The first step in calculating the SIP control requirement is to list the ozone maxima and dates of the five highest ozone days at each site. A site is only included for a specific day if the wind data indicate that the site is actually downwind of the urban area.

An examination of the high days at each site reveals some duplication in the dates of high ozone days among sites. For example, in Table 2.2, June 8 appears for both Site A and Site B. For this case, the same isopleth diagram can usually be used at each site. Control estimates are then made for each site/day combination using the appropriate ozone isopleth diagram.

Experience with the model, and an examination of the differences in such factors as transported ozone levels between the day to be modeled and other days with higher ozone maxima, may provide a means for limiting the number of sites or the number of isopleth diagrams to be generated for each site. In the example in Table 2-2, because of the duplication of days among the sites, only two isopleth diagrams were generated for the Site A, and only one for Site C. Then, using the selection criteria presented in Table 2-1, the site-specific control requirements were obtained (the control estimates enclosed in boxes in Table 2-2). In Table 2-2

Table 2-2. Selecting the SIP Control Requirement: An Example

Site A			Site B			Site C**		
O_3+	Date	% R	O_3+	Date	% R	O_3+	Date	% R
.24	10/1/80	60	.22	6/8/81	58	.16	7/31/81	45
.18	6/8/81	57	.19	8/25/80	54	.15	9/17/81	(38)
.16	10/2/80	(45)	.19	10/2/80	55	.15	6/1/81	*
.15	8/13/81	39	.18	8/26/80	(51)			
.14	8/21/80	*	.17	7/26/79	49			

SIP Control Requirement = 51% obtained from Site B.

* Isopleth diagrams were not generated for these days since transport and mixing heights were similar to days with significantly higher ozone values; thus, the control requirements would be less.

** On these days, the Site C was actually downwind of the city as indicated by local wind data.

\+ The daily maximum O_3 at each site.

Assumptions: (1) Urban Area has three monitoring sites, Site A, Site B and Site C.

(2) Site A has two years of ozone data, Site B has three years of data, and Site C has only one year of ozone data.

(3) Control requirements (%R) may not decrease monotonically due to daily variations in transported ozone levels, mixing heights, NMOC/NO_x ratios, etc.

the SIP control requirement is the maximum of the site specific control requirements, i.e., the 51 percent estimate Site B for this example.

In summary, the method for estimating urban area control requirements for 1982 SIPs involves (1) the repeated application of the OZIPP model to generate isopleth diagrams for each of the five highest ozone days from the past three years at each site, (2) the use of the EKMA procedure to provide a control estimate for each site-day, and (3) the selection of the SIP control requirement as the control estimate needed to demonstrate attainment at all monitoring sites for the urban area as a whole.

3.0 GENERATION OF DAY-SPECIFIC ISOPLETH DIAGRAMS

As described in Section 2.1, a number of days with elevated ozone concentrations are selected for modeling. An ozone isopleth diagram is generated for each day using the OZIPP computer model. Each model application requires the use of day-specific modeling inputs. Day-specific empirical data (or suitable surrogates) are then used in conjunction with each diagram to calculate the VOC and/or NO_x controls necessary to reduce the peak hourly ozone concentrations observed on each day to 0.12 ppm. The empirical data are used to locate a starting point on each diagram, from which control calculations are made. Because the scales of the diagram axes can be varied in OZIPP, the empirical data must be developed prior to generation of a diagram to insure that the starting point is located in an appropriate position on the diagram. This Chapter describes the methodologies appropriate for deriving the day-specific modeling data, the day-specific empirical data, and the procedures for generating the diagrams. The control calculations are described in Chapter 4.

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In describing the techniques for developing modeling inputs, more than one procedure is usually presented. The first method listed is generally preferable, given the level of detail of information normally available. However, it is recognized that in some instances more detailed information may be available and could be included in the analysis, if desired. On the other hand, information may not always be available, or reliable. Consequently, optional methods of developing input data are also presented. If no information at all is available, default values, or methods, are sometimes included. In practice, the methods used to derive input to the model involve a trade-off between the resources required to collect and process data, and the enhanced credibility of the analysis

by more completely representing physical processes. The preferred approaches are designed to provide a fairly complete representation, given data assumed to be commonly available. To insure specificity to a particular city under review, city-specific determinations of input data are strongly recommended, with default measures recommended only as a last resort.

3.1 OZIPP MODELING DATA

The conceptual basis for the OZIPP/EKMA model has been described References 1, 2 and 3. The following discussion focuses on the procedures for deriving the input data for using OZIPP to generate isopleth diagrams for each day investigated.

As shown in Figure 3.1, ozone isopleths are expressed as explicit functions of initial NMOC and NO_x concentrations. However, the positioning of the ozone isopleths on the diagram is also an implicit function of meteorology, pollutant transport, emissions, and chemistry. In the OZIPP model, several variables can be input to the model to tailor the diagram to a specific situation, i.e., the atmospheric conditions occurring on that day. The OZIPP input variables for developing day specific diagrams can be grouped according to the following categories:

1) light intensity
2) dilution
3) O_3 transport
4) precursor transport
5) emissions
6) reactivity

In the discussion that follows, procedures for deriving the input variables in each group are described.

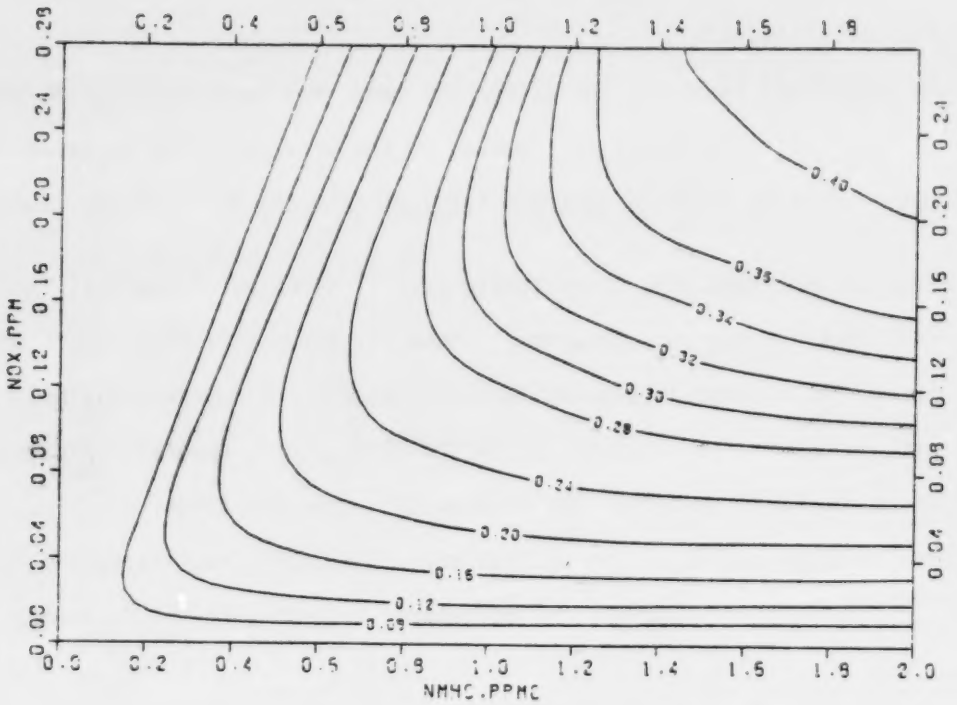

Figure 3-1. Example Ozone Isopleth Diagram.

3.1.1 Light Intensity

The OZIPP program utilizes latitude, longitude, day of the year, and time zone to calculate the appropriate variation of photolytic rate constants. The model does not provide for adjusting the attenuation of light intensity due to cloud cover. Hence, conditions without significant cloud cover are assumed, corresponding to the types of conditions normally found on days with high ozone concentrations. Studies have shown that control requirements are relatively insensitive to variations in light intensity, so this assumption is not perceived as critical.[10]

Recommended Procedure: The recommended approach for specifying light intensity is straightforward. The local latitude and longitude for the center of the city should be used. The day of the year and the appropriate time zone should be specified, as described in EPA 600/8-78-014a.[3]

3.1.2 Dilution

In OZIPP, dilution is assumed to occur as a result of the rise in atmospheric mixing height which normally occurs between early morning and mid-afternoon. The mixing height is the top of a surface-based layer of air which is well-mixed due to mechanical and thermal turbulence. The mixing height rise is governed by the specification of four variables input to OZIPP: the 0800 local civil time (LCT)* mixing height, the maximum mixing height, the time at which the rise begins in the model (e.g., 0800 LCT), and the time at which the mixing height reaches its maximum.

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* In most areas in the United States, local civil time is identical to local daylight time during the ozone season. In areas which do not switch to daylight savings time, local civil time is the same as local standard time. The OZIPP program was designed to operate on the basis of Local Daylight Savings Time. For those areas which do not switch to daylight savings time, the model may be made to operate on standard time by adding one (1) hour to the time zone described in Section 3.1.1. See also page 39 of Reference 3.

Recommended Procedure: The recommended approach for estimating the 0800 LCT mixing height and the maximum mixing height uses temperature sounding data routinely compiled by the National Weather Service. Supplemental surface temperature and pressure data are also needed. Table 3-1 contains guidelines for selecting the required data, while the detailed procedures for calculating the morning and maximum mixing heights are contained in Appendix A. A minimum 0800 LCT mixing height of 250 meters above ground level (AGL) is recommended. This value is based on studies of the St. Louis and Philadelphia early morning urban mixed-layer,[11] and is recommended even if the morning mixing height computed using the NWS sounding is lower. The 250 m minimum is due to mechanical turbulence caused by increased surface roughness in the urban area. Also, any maximum mixing height greater than twice the climatological value contained in Table A-1 of Appendix A or Reference 12 should be checked as described in Appendix A. If no alternate data are available in this case, twice the climatological value is recommended in place of the computed value.

Alternate Procedure: Direct measurements of the urban vertical temperature profile may be used in place of the NWS data if they are available. Mixing heights can be found from local urban radiosonde measurements, helicopter soundings, or by sodar (i.e., acoustic radar). Identical computational procedures as those described in Section A-2 of Appendix A should be employed. As for the recommended procedure, a minimum value of 250 meters should be used if the computed morning mixing height is less than 250 meters.

Default Procedure: If none of the information needed for the first two procedures is available, then the climatological values listed in Table A-1, or obtained from Reference 12 may be used. If the latter is used, the average summertime maximum mixing height on non-precipitation days should be used. For the default procedure, the mixing height rise may be assumed to continue from 250 meters at 0800 LCT until the time of the climatological maximum daily surface temperature. If the latter is unknown, then a climatological value of 1500 LDT (i.e., 1400 LST) can be assumed.

3.1.3 Transport of Ozone

The transport of ozone and its precursors into and from urban areas has been reported by numerous investigators.[1,13-16] The discussion in this section is limited to the transport of ozone; precursor transport is discussed in the following section.

The two primary mechanisms by which ozone is transported into an urban area are:

Table 3-1. Data Requirements For Calculating Mixing Heights According to the Recommended Procedure

1. Surface Temperature Measurements - For each day modeled, the urban surface temperature at 0800 LCT and the maximum temperature occurring between 0800 and 1800 LCT are required. The most suitable data are those taken from a well ventilated shelter at a site near the center of the urban area.

2. Surface Atmospheric Pressure Data - For each day modeled, the urban surface barometric pressures for the same time and location of the temperature measurements are needed. If these are not available, local National Weather Service (NWS) or Federal Aviation Administration (FAA) pressure data may be used.

3. NWS Radiosonde Data - For each day modeled, mixing heights are calculated from vertical temperature profiles obtained from radiosondes taken by the NWS at several sites throughout the United States. Appendix A contains information on selecting an appropriate site and obtaining the necessary data.

1) advection of ozone along the earth's surface, and

2) advection of ozone aloft, typically at night and during early morning hours above the ground-based mixed layer, with downward mixing when the mixing layer increases later in the day.

Ozone transported at the surface is subject to surface reactions and scavenging by other species (e.g., NO) emitted during the night. As a result of nighttime atmospheric stability, ozone transported aloft does not come into contact with scavengers emitted during the night. Thus, overnight advection of ozone aloft appears to be the more significant mechanism of transport from one urban area to another.[1,13]

Control strategies designed to attain and/or maintain the ozone standard in individual urban areas must take into consideration the impact of transported ozone on peak afternoon concentrations. The procedure of using OZIPP with the EKMA technique for the case where future transported ozone concentrations might be significantly different from current levels is explained fully in References 1 and 3, and described in Chapter 4 of this report.

A. Present Transport of Ozone at the Surface

The chief impact of ozone transport near the surface is expected to be the more rapid conversion of NO to NO_2. When incoming ozone near the ground was varied using OZIPP, the impact on maximum ozone concentrations was generally found to be negligible. This finding held true for incoming concentrations as high as 0.12 ppm ozone.[2] In addition, several field studies have shown that ozone transported along the surface tends to be minimal.[13,14,17]

Recommended Procedure: Based on the previous discussion, it is recommended that, for most situations, the value for present ozone transported at the surface be set equal to zero for each day modeled.

Alternate Procedure: If the situation arises, as a result of the geographical location of the city under study, that consideration of surface ozone transport is desirable, then daily estimates of ozone surface transport may be obtained from urban monitoring sites. It is suggested that the 6-9 a.m. LCT average ozone concentration at an urban site(s) be used as the estimate of the concentration of ozone transported into the urban area along the surface for the given day.*

B. Present Transport of Ozone Aloft

As noted above, it appears that unscavenged ozone transported aloft is likely to be the component of transport having the greatest impact on maximum afternoon ozone levels observed within or downwind from cities. Thus, daily estimates of ozone aloft are needed for control strategy development with OZIPP/EKMA. Techniques for estimating the level of ozone transported aloft have been the subject of two studies.[13,18] Five different techniques, which were considered to be feasible were field tested in Philadelphia during the summer of 1978.[13] The five methods are: 1) use of fixed ground based stations; 2) use of airborne measurements in a dedicated aircraft; 3) use of airborne measurements with a portable instrument package; 4) use of free lift balloon soundings; and 5) use of soundings by tethered balloon. Reference 13 contains a detailed description of each of these techniques as well as a discussion of the findings of the study. Of the five measurement techniques evaluated, surface measurements at fixed sites, airborne measurements by dedicated instrumented aircraft and soundings by ozonesonde beneath a free balloon were judged to be practical means of providing information on ozone transported aloft.

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* See related footnote on page 39

Recommended Procedure: In selecting the technique to use, consideration was given to such factors as technical capability and available funding, and the intended use of the data. Ozone measurements taken on the day being modeled are recommended as the best estimate of ozone aloft. These measurements should be obtained at surface monitoring sites upwind of the city during the first hour after breakup of the nocturnal inversion. An acoustic radar (sodar) can be used to determine the time of inversion breakup for the day. If the time of the breakup of the nocturnal radiative inversion is not known, the 1000-1200 Local Standard Time average ozone concentration recorded at the upwind monitor should be used as the transport estimate. A major advantage of surface measurements is that it is the only method which allows continuous measurements, and thus assurance that measurements exist for days or for times of day which are later determined to be of interest. The site(s) should be located in as rural a location as possible so as not to be appreciably affected by local sources of precursors. The distance such upwind sites should be located from a city depends on the extent of urban development. Because it is desirable not to measure pollutants which are recirculated from the city under review, a distance of 40 km or more upwind from the urban core should be sufficient. This distance perhaps could be reduced for smaller cities. Figure 3-2 depicts orientations for acceptable upwind sites.

Alternate Procedure: Information on the vertical distribution of ozone transported above the surface layer in the early morning may be used directly if it is available. Such information might include aircraft or free-lift ozonesonde measurements. The reader is referred to Reference 13 for a detailed discussion of these techniques.

Missing Data: In the event that an estimate of transport is not available for a given day being modeled, the median transport value from the remaining days being modeled should be used as a default value. This procedure applies to all the data gathering techniques described above; fixed site, aircraft and ozonesonde observations.

3.1.4 Precursor Transport

Just as for ozone, precursor pollutants could be transported in both the surface layer and aloft. However, consideration of precursor transport is usually not considered essential for several reasons. First, transported precursor concentrations tend to be substantially less than concentrations within urban areas.[2] Secondly, in most areas transported organic species are likely to be less reactive than urban species because of the rapid reactions of the more reactive species.

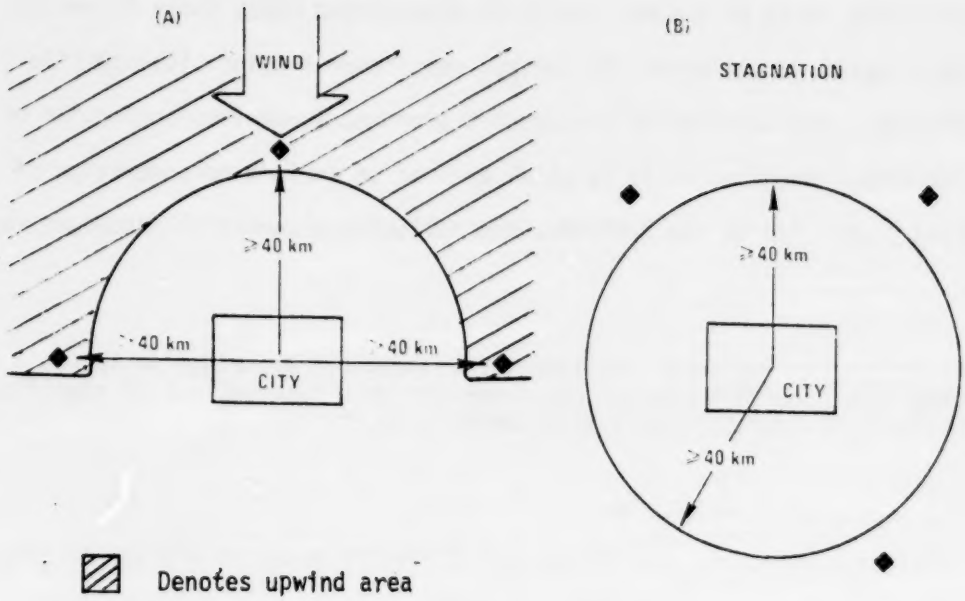

Figure 3-2. Examples of acceptable monitoring locations for estimating transported ozone.

Recommended Procedure: Several studies have suggested that significant transport of precursors into an urban area is not an important consideration in most cases.[2,13,18] Consequently, transported concentrations of NMOC and NO_x, in both the surface layer and aloft, are recommended to be set to zero.

Sensitivity studies presented in Appendix B and elsewhere[2] indicate that, for a wide range of assumed levels of transported NMOC, there is not an appreciable impact on estimated VOC control requirements using city-specific EKMA. Further, consideration of transported precursors requires collection of additional data. However, if it is still desired to include consideration of transported precursors in the analysis, the following alternative procedure may be used.

Alternate Procedure: Utilize the methodology presented in Appendix B to estimate local emission control requirements for a city subject to significant and pervasive precursor transport from upwind sources.

3.1.5 Post 8 a.m. Emissions

As was previously described, the OZIPP/EKMA model is similar in concept to a Lagrangian photochemical dispersion model in that ozone and precursor concentrations within a well mixed column of air are modeled as the column traverses the city. The column of well-mixed air is assumed to originate in the urban core, and begin moving at 0800 LCT toward the site of the peak ozone concentration. Thus, the emissions occurring subsequent to 0800 LCT are determined by the space-time track of the column. Within OZIPP, emissions data are input to the model for each hour after 0800 LCT, and are expressed relative to the initial concentrations. Thus, there are two basic, and separate, problems in deriving the necessary emissions information:

1) determining emissions along the space-time track of the theoretical column;

2) expressing the emissions derived in 1) relative to the initial concentrations. These initial concentrations are assumed to be the result of local urban emissions occurring prior to 8 a.m.

The first of these involves the use of an emissions inventory to estimate the emissions occurring along the assumed path. The second involves the calculation of relative emission fractions that are directly input to the OZIPP model. Each of these is discussed separately below.

A. Preparation of Emissions Data

The first step in preparing the available emissions data for use in OZIPP/EKMA is to specify the space-time track of the column trajectory. The column is assumed to begin moving from the urban core at 0800 LCT directly towards the site of the peak ozone concentration. The rate of movement is estimated using the time and location of the peak ozone concentration. The column is assumed to move at uniform speed (throughout the day) to the site of the peak ozone value such that it arrives at that site at the time of the observed peak.* For example, assume the observed peak one-hour-average ozone concentration on a particular day was measured between 1400-1500 LCT at a site 35 kilometers downwind of the urban core. The column speed would be calculated

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* Recall from Chapter 2 that some duplication in high ozone days is likely for many of the sites in the monitoring network. A rigorous modeling approach would involve specifying trajectories for each site/day combination, and generating the corresponding diagrams. However, in most instances, the trajectory leading to the peak ozone observed on that day should be a sufficient approximation of the other trajectories. Hence, only one diagram can be developed for the day and be used for all sites. The exception would be cases in which significantly different post 8 a.m. emissions occur along the different trajectories between the urban core and the different monitoring sites. For this situation, separate site/day diagrams need to be developed.

by dividing 35 kilometers by seven hours (i.e., the elapsed time between 0800 LCT and 1500 LCT). The location of the column at any particular hour would be determined by assuming the column moved in a straight line between the urban core and the site of the peak at the uniform speed. (For the example, the speed would be 5 km/hour.) The assumed trajectory may not be identical to the actual trajectory corresponding to highest observed ozone concentrations. However, the wind data should be checked to assure the modeler that the peak ozone concentration observed at a monitor station is, in fact, downwind from the city. Observation of urban NMOC/NO_x ratios made during the St. Louis RAPS do not suggest the prevailing urban ratio varies greatly during the morning. Further, several hours are required for ozone to reach its peak. Hence, the trajectory described above should be an acceptable approximation, provided the column of air passes over the city by mid-morning (e.g., 1000-1100 LCT).

With the trajectory path identified, the next step in preparing the emissions data is to use the emission inventory to calculate the hourly emissions. The procedure depends to some degree on the spatial and temporal resolution of the emission inventory. In the recommended methodology that follows, a seasonally adjusted, annual county-wide emissions inventory of reactive VOC* and NO_x is assumed to be available. This level of detail will result using procedures presented in Reference 19. An alternate method addresses procedures that can be used with inventories of greater temporal and/or spatial

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* In the discussion of post 8 a.m. emissions in Section 3.1.5, the term "VOC," volatile organic compounds, refers to the sum of reactive organic emissions included in emission inventories. The term "NMOC," non-methane organic compounds, refers to ambient measurements of all organic compounds other than methane.

resolution. Regardless of the resolution of the inventory, the goal of this step is to develop emission densities representative of the area over which the column is assumed to pass each hour. Thus, the emission density represents the average emission density "as seen by the column" for each hour between the simulation start and the time of the measured peak.

Recommended Procedure: For this approach, a county-wide emissions inventory is assumed; i.e., total reactive VOC and NO_x emissions on a seasonally adjusted annual basis are available at the county level only. The simplest method of deriving the necessary information is to compute the county-wide emission density by summing total emissions (point plus area source) and dividing by the area of the county. Hourly resolution of the inventory can be estimated by assuming emissions occur uniformly throughout the year. For example, one would divide the seasonally adjusted annual emissions by 8760 hrs/yr. The emission density at any hour is thus determined by the county in which the trajectory path is located for that hour. For those hours in which the trajectory path crosses a county boundary(s), the county emission densities may simply be averaged.

The procedure just described can best be illustrated by example (see Figure 3-3). Part A of the figure shows the information typically available. Here it assumed that the peak ozone concentration measured on the example day occurred at a site 35 kilometers downwind of the urban area between 1400 and 1500 LCT. The first step is to depict the trajectory path on an appropriate map by marking off hourly segments (see Part B). Step 2 involves deriving the county-wide emission densities on an hourly basis (Part C). Finally, in Step 3, the sequence of emissions is determined by using the emissions for the county in which each hourly segment lies. For those cases in which a segment lies in two counties, the emission densities of the two counties were averaged. Part D shows the results of Step 3.

The approach just described is a relatively simple one which is consistent with the amount of information typically available. However, as

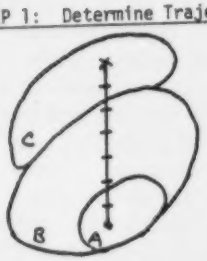
A) Information Available

Peak ozone measured between 1400-1500 LCT. Site is 35km downwind of center-city (cc).

County Emissions Data

County	Area, km^2	Adjusted VOC Emissions kg/yr	Adjusted NO_x Emissions kg/yr
A	150	5.45×10^7	2.96×10^7
B	500	3.93×10^7	3.38×10^7
C	300	1.68×10^6	1.17×10^6

B) STEP 1: Determine Trajectory Segments



A straight line is drawn between the center-city and the downwind site. The line is divided into seven equal segments, representing the number of hours between 800 and 1500 LCT.

C) STEP 2: Calculate, hourly, county-wide emission densities

County	Area, km^2	Adjusted VOC Emissions kg/yr	Adjusted VOC Emission* density, kg/hr km^2	Adjusted NO_x Emissions kg/yr	Adjusted NO_x Emission* density, kg/hr km^2
A	150	5.45×10^7	41.5	2.96×10^7	22.5
B	500	3.93×10^7	9.0	3.38×10^7	7.7
C	300	1.68×10^6	.6	1.17×10^6	.4

*Emission density = emissions/(8760 x area)

D) STEP 3: Specify Sequence of Emission Densities

Hour	Time, LCT	Trajectory Segment Location (County)	Adjusted VOC Emission density, kg/km^2 hr	Adjusted NO_x Emission density, kg/km^2 hr
1	8-9	A	41.5	22.5
2	9-10	A/B	25.3	15.1
3	10-11	B	9.0	7.7
4	11-12	B	9.0	7.7
5	12-13	B	9.0	7.7
6	13-14	B/C	4.8	4.1
7	14-15	C	.6	.4

Figure 3-3. Example Formulation of Post 8 a.m. Emission Densities Scheme

described below, more sophisticated techniques may sometimes be desired. It should be remembered, however, that city-specific EKMA (Level III analysis) does not require a precise definition of an air parcel trajectory. Use of spatially and temporally detailed inventories implies a need for greater efforts to define trajectories. Such efforts are more consistent with the use of more sophisticated models. Although the use of very detailed emission inventories is inconsistent with the degree of sophistication inherent in city-specific EKMA, methods for improving spatial and temporal resolution are possible. These are described in the following paragraphs.

Alternate Procedure: In the recommended approach, emission densities were determined on a county-wide basis. In some instances, a finer spatial resolution may be desired. For example, suppose total emissions are available for the county, but the county encompasses a very large land area, of which the urban area is a relatively small part. In this case, one may wish to suballocate the emissions to areas smaller than the county levels. For example, the very large county might be divided into a rural portion and an urban portion, with emissions apportioned to each area. The methodology for apportioning will usually depend on available data and the particular situation encountered. Consequently, no specific guidance can be given here, but the concepts contained in References 19 and 20 may be adopted. If an allocation is performed to a sub-county level, the sub-county areas should not be resolved to less than 100 square kilometers. Resolution to smaller areas is not recommended because of the inability of the model to consider horizontal gradients in pollutant concentrations.

Alternate Procedure: A second way in which the recommended approach could be made more precise is more detailed consideration of the temporal distribution of emissions. In the recommended approach, hour by hour differences in emissions are not considered. If more detailed information is available, these data could be employed to derive more precise temporal resolution of emissions as described in Reference 20. In the absence of geographically specific data, a city-wide average may generally be used for distributing temporal emission patterns. For example, the distribution could be calculated as the average of the temporal distribution of mobile and stationary sources.

Alternate Procedure: In some cases, emissions inventory data will be available that is of a finer resolution than a county-wide/annual basis. For example, an hourly gridded emissions inventory may be available. This procedure addresses the problem of using an hourly emissions inventory with grids finer than 10x10 kilometers on a side. However, the development of a gridded inventory specifically for use with the OZIPP/EKMA technique is not recommended.

Recall that the model underlying the OZIPP/EKMA procedure does not consider the existence of horizontal concentration gradients. The emission density "seen by the column" during any hour should represent an average. Consequently, it is recommended that emissions inventory data resolved to grids smaller than 10x10 kilometers (i.e., 100 km^2) be aggregated to a minimum size of 100 square kilometer grids. The larger grid squares conform more readily to the assumptions underlying the model. The larger grid cells should be located such that the average emission density is representative of the area it covers. Thus, for example, a 10x10 km grid square might be centered on the center city, and the new grid network for OZIPP/EKMA developed from there.

The procedure for determining the emissions encountered by the column of air simulated with OZIPP is similar to the one described for the recommended methodology. However, in this case the network with the larger grid squares is used in place of the county-wide data. The resulting emissions schedule is established by the location of the trajectory segments with respect to the grid cells. If a trajectory segment crosses a grid boundary, the emission densities of the adjacent grids may be averaged.

B. Derivation of Emission Fractions

In Section A, the procedure for estimating the sequence of emissions was described. The emission sequence represents emissions injected into the modeled column of air each hour subsequent to the 0800 LCT simulation starting time. As indicated in the example problem (see Figure 3-3), the emission densities comprising the sequence of emissions are expressed in terms of mass per unit area (e.g., kg/km^2). In OZIPP, however, the emissions must be expressed relative to initial concentrations. Thus, it is necessary to translate the sequence of emissions (in mass units) to fractions of initial concentrations. This is accomplished by first deriving an initial emission density which is tied to the initial concentration. The emission fractions are then computed by dividing the hourly post 8 a.m. emission densities (i.e., from the sequence of emissions) by the initial emission density. In essence, this procedure is the same as calculating the concentrations that would be generated by the emissions within the imaginary column of air after one hour, and then dividing those computed

concentrations by the initial concentration to obtain the appropriate fractions.

The approach recommended for computing emission fractions is one in which an initial emission density is computed from initial conditions. The initial emission density is calculated as the emission density necessary to generate in one hour the initial concentrations observed within the column. So, if an initially empty column were "exposed" to the calculated initial emission density for one hour, the concentrations of precursors in the column at the end of the hour would equal the observed initial level. The emission density for any hour after 0800 LCT can then be related to the initial concentrations by means of the initial emission density. For example, if the emission density for hour 1 (i.e., 0800-0900 LCT) is one-third that of the initial emission density, then one-third of the initial concentration would be generated by the emissions for that hour. The emission fraction can therefore be calculated using the following equations:

$$Q_o = \alpha\, C_o\, H_o \qquad (3\text{-}1)$$

and

$$E_i = \frac{Q_i}{Q_o} \qquad (3\text{-}2)$$

where

Q_o = calculated initial emission density (kg/km^2)

C_o = initial precursor concentration (ppm)

H_o = initial mixing height (kilometers)

Q_i = emission density for hour i from the sequence of emissions (kg/km^2)

E_i = emission fraction for hour i

α = conversion factor for converting from volumetric to mass units

The methodology is further illustrated in Figure 3-4, and the procedures for deriving the necessary data are described below.

Recommended Procedure: The first step in calculating the emission fractions is to compute an initial emission density for NO_x and VOC. This requires the specification of an initial concentration for each precursor and the initial mixing height. The initial concentrations can be obtained from ambient 6-9 a.m. measurements of NMOC and NO_x on the specific day being modeled. If NMOC or NO_x ambient data for the specific day being modeled are unavailable, then the median 6-9 a.m. NMOC and NO_x concentration for all days being modeled should be used for each precursor.

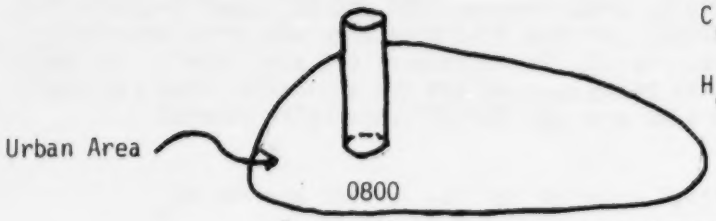
The computational steps necessary to calculate the emission fractions are outlined in Table 3-2 and illustrated in Figure 3-5. A brief explanation of each step follows:

Step 1: The initial concentration to be used in the emission fraction calculations is the 6-9 a.m. average precursor concentration in the urban area. (Average concentrations are calculated for both NMOC and NO_x.) The procedures for calculating the 6-9 a.m. average concentrations at individual monitors are described in Section 3.2.2, and should be followed here. If more than one monitor is located in the urban area, the 6-9 a.m. concentrations at each monitor should be averaged to obtain an the overall urban average 6-9 a.m. concentration.

Step 2: An initial emission density is calculated for VOC and NO_x, individually. The recommended conversion factors (α) for VOC and NO_x are 595 kg HC/ppmC km^3 and 1890 kg NO_x/ppm km^3, respectively. The derivation of the conversion factors is described in Table 3-2. For converting NMOC to VOC, it is assumed that one ppmC represents a molecular weight equivalent to $CH_{2.5}$[9]. For NO_x, a molecular weight of 46 is assumed because inventories list NO_x as equivalent NO_2.

Step 3: The hourly emission fractions are calculated by dividing the emission densities for each hour by the initial emission density. This is done separately for each pollutant.

Time: 0800

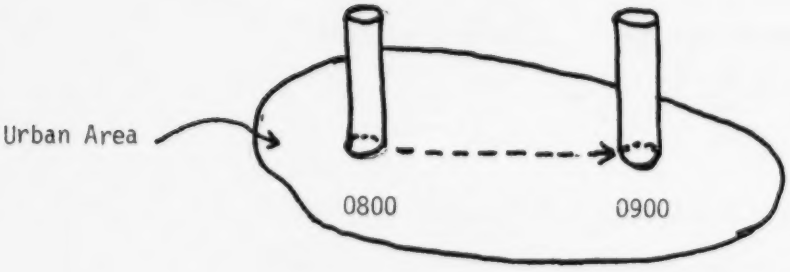


C_o = Column concentration at 0800 LCT

H_o = Mixing Height at 0800 LCT

Assume the precursor concentration in the column is C_o. Therefore, $Q_o = C_o H_o$

Time: 0800 - 0900



Assume the emission density for the hour 0800-0900 equals 1/4 of the emission density calculated from the initial concentration.

The concentration generated by the emissions occurring between 0800 and 0900 would be 1/4 of the initial concentration.

Therefore, the emission fraction for Hour 1 would be 1/4, or .25:

$$E_i = \frac{Q_i}{Q_o} = .25$$

Figure 3-4. Illustration of Emission Fractions Calculated Using Initial Conditions.

Table 3-2. Recommended Procedure For Calculating Emission Fractions

Step 1: Calculate the 6-9 a.m. urban average NMOC and NO_x concentrations for the day being modeled. If data from more than one urban monitoring site are available, average the individual 6-9 a.m. levels. If data for the specific day being modeled are not available, then use the median of the 6-9 a.m. averages for all days being modeled.

Step 2: Calculate the initial emission density for VOC and for NO_x:

$$Q_o = \propto C_o H_o$$

where

Q_o = Initial emission density, kg/km^2

H_o = Day-Specific mixing height at 0800 LCT (kilometers)

$\propto$ = Conversion factor*

Step 3: Calculate individual hourly emission fractions:

$$E_i = \frac{Q_i}{Q_o}$$

where

E_i = Hourly emission fraction for hour i

Q_i = Emission density for hour i, kg/km^2

Q_o = Initial emission density calculated in Step 2 above, kg/km^2

---

* Conversion factors: $\propto$ For NMOC to VOC = 595 kg/km^3 ppmC

$\propto$ For NO_x = 1890 kg/km^3 ppm

These conversion factors were calculated assuming a molar density of dry air at 25°C (i.e., 1 mole/24.4 liters). For NMOC to VOC conversion, the molecular equivalent to one ppmC is assumed to be $CH_{2.5}$ (i.e., a molecular weight of 14.5 is assumed).[9] For NO_x, a molecular weight of 46 is assumed since NO_x emission inventories are compiled as equivalent NO_2).

A) Available Information

	Urban Monitor	Pollutant	6-7	7-8	8-9	6-9 AVG.
• Air Quality Data						
NMOC [=] ppmC	1	NMOC	2.3	2.0	1.5	1.9
NO_x [=] ppm		NO_x	.250	.200	.180	.210
	2	NMOC	1.7	1.7	1.6	1.7
		NO_x	.190	.210	.170	.190

• Emissions Schedule Shown In Figure 3-3

• 0800 LCT Mixing Height = .25 km

B) Step 1: Calculate Urban Average 6-9 LCT Concentration

$$\bar{C}_{NMOC} = \frac{1.9 + 1.7}{2} = 1.8$$

$$\bar{C}_{NO_x} = \frac{.210 + .190}{2} = .200$$

C) Step 2: Calculate Initial Emission Densities

For VOC

$$Qo = a\ Co\ Ho = (595\ ^{kg}/_{km^3}\ ppmC)\ (1.8\ ppmC)\ (.25\ km) = 268\ ^{kg}/_{km^2}$$

For NO_x

$$Qo = \alpha\ Co\ Ho = (1890\ ^{kg}/_{km^3}\ ppm)\ (.200\ ppm)\ (.25\ km) = 95\ ^{kg}/_{km^2}$$

D) Step 3: Calculate Hourly Emission Fractions

Hour	Time, LCT	VOC Hourly Emission Density,* kg/km²	NMOC Emission Fraction**	NO_x Hourly Emission Density* kg/km²	NO_x Emission Fraction**
1	8-9	41.5	.15	22.5	.24
2	9-10	25.3	.09	15.1	.16
3	10-11	9.0	.03	7.7	.08
4	11-12	9.0	.03	7.7	.08
5	12-13	9.0	.03	7.7	.08
6	13-14	4.8	.02	4.1	.04
7	14-15	.6	.00	.4	.00

* Hourly Emission Densities From Figure 3-3

** Emission Fraction = (Emission Density)/(Initial Density)

Figure 3-5. Example Calculation of Emission Fractions

3.1.6 Reactivity

The OZIPP model incorporates a chemical kinetic mechanism to describe the reactions taking place among pollutants. The kinetics model used in OZIPP represents a detailed sequence of chemical reactions which has been proposed for a mixture of propylene, n-butane and NO_x. The chemical mechanism used in the kinetics model is based on information obtained in smog chamber experiments with propylene and n-butane separately.[22, 23] The kinetics model predictions were matched against Bureau of Mines (BOM) smog chamber data obtained by irradiating automobile exhaust.[24] Initial proportions of propylene and n-butane were then adjusted so that consistently close agreement was obtained with observations in the BOM chamber. Of the available smog chamber studies, the ones using automotive exhaust are thought to use a mix of reactants most representative of the mixes found in urban atmospheres.

In OZIPP, total NMOC is represented by the sum of propylene and n-butane, with aldehydes related to the total "NMOC" concentration. The reactivity is determined by specification of three variables: 1) the fraction of NMOC that is propylene; 2) the fraction of NMOC that is to be added as aldehydes; and 3) the fraction of initial total NO_x that is NO_2. The proportional mix of propylene and n-butane for which OZIPP yields peak ozone predictions comparable to that observed with automobile exhaust in the BOM chamber is 25 percent and 75 percent, respectively, with an additional 5 percent of the initial NMOC added as aldehydes. Propylene-butane mixes have not been established for any atmospheric mix other than the automotive mix used in the BOM chamber. Unless satisfactory correspondence between other atmospheric mixes and other propylene-butane mixes can be established, the 25 percent propylene, 75 percent butane, plus 5 percent aldehydes, should be used.

The third variable to consider is the fraction of the initial NO_2 that is NO_x. Sensitivity studies have suggested that the effect of the initial NO_2/NO_x mix on peak ozone concentrations is small.[10] Consequently, specification of this variable is not deemed critical.

Recommended Procedure: The 25 percent propylene-75 percent butane mix, with 5 percent of the initial NMOC added as aldehydes, should be assumed for the model simulations. This mixture corresponds to the reactivity of automotive exhaust irradiated in a smog chamber. Unless satisfactory correspondence can be established between other propylene-butane mixes and other atmospheric mixtures which differ appreciably from automotive exhaust, the 75 percent/25 percent mix should be used.

A default value of 25 percent for the initial NO_2 to NO_x ratio is recommended. Sensitivity studies have shown that peak ozone concentrations (and hence control estimates) are relatively insensitive to any particular assumption. However, day-specific information may be used if desired. For this case, the 6-9 a.m. average NO_2 should be divided by 6-9 a.m. average NO_x to obtain an NO_2/NO_x ratio at each monitor located in the central core of the urban area. If more than one monitor is located in the urban area, then an average ratio may be obtained by averaging the individual ratios.*

3.2 EMPIRICAL DATA

Two pieces of empirical data are needed to establish a starting point on the ozone isopleth diagram for calculating control requirements. The first is the maximum one-hour average ozone concentration observed at the site of interest. The degree of emission control necessary to reduce this "peak" to 0.12 ppm is to be calculated; hence, the peak level will be termed the daily design value.

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* Strictly speaking, this latter procedure is more consistent with the use of measured 6-9 a.m. urban ozone concentrations to estimate ozone transported into the city within the morning mixed layer (see page 23). However, use of the default value makes little difference in the resulting control estimates.

The second piece of information needed is the NMOC/NO_x ratio. This ratio is derived from the 6-9 a.m. concentrations of NMOC and NO_x within the urban area. These measurements correspond conceptually to the NMOC and NO_x concentrations on the axes of the isopleth diagrams. The ratio will be termed the design ratio. The procedures for deriving both the design ozone values and the design ratios are described below.

3.2.1 Daily Ozone Design Value

The daily ozone design value is used in conjunction with the NMOC/NO_x ratio to establish a starting point on the isopleth diagram for calculating control estimates. The "daily design value" is used to refer to the measured maximum hourly ozone value for the day being modeled.* For use with the isopleth diagram, the design value should be expressed in ppm units rounded to two decimal places.

Recommended Procedure: A daily maximum 1 hour value is obtained for each site which is downwind of the city, and/or within the city in the case of light and variable winds on the day for which the isopleth diagram is to be developed. Surface wind data should be examined to assure that the site is not "upwind" of the city. Based on the results of field studies and reviews in which ozone gradients downwind from urban areas were examined, peak ozone concentrations should generally be observed within 15-45 km downwind of the central business district.[2,25-26] Specific siting criteria for the monitoring of photochemical pollutants are discussed elsewhere.[2,26-27]

3.2.2 NMOC/NO_x Ratios

The prevailing 6-9 a.m. LCT NMOC/NO_x ratio measured in the urban core of the city is the second piece of empirical data required to define the starting point on the isopleth diagram. The design ratio is viewed as a characteristic of

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* Note that an ozone design value exists for each site for which the day being modeled is among the five highest ozone days.

the city which would prevail during the remainder of the morning and early afternoon in the absence of chemical reactions. The ozone isopleth diagram expresses peak ozone concentrations as a function of the initial concentration of NMOC and NO_x. Thus, the 6-9 a.m. LCT NMOC/NO_x ratio is considered to be the appropriate ratio for use with the isopleth diagram since this ratio is consistent with the conceptual basis of the model.[28] To ensure that representative ratios are obtained, the NMOC and NO_x instruments should be collocated in the central core of the urban area. The site(s) should be located in an area of relatively uniform emission density and not significantly influenced by any individual source. More detailed guidance on siting NMOC instruments is contained in Reference 29. Guidance on the operation of NMOC instruments is available in Reference 30.

Significant discrepancies have been found between NMOC/NO_x ratios calculated on the basis of ambient measurements and those obtained from emission inventory data.[31] Reasons for the lack of correlation between the two ratio calculation procedures have not been resolved. As a result, only ambient NMOC/NO_x ratios should be used with EKMA since these ratios are consistent with the conceptual basis of the model and the emission ratios have been shown to be poor surrogates for these ambient ratios. To ensure maximum usefulness of the continuous NMOC data, careful attention to calibration, operational procedures, and quality assurance is necessary. Presently available instruments are capable of yielding acceptable data at concentrations above about 0.5 ppmC if they are carefully maintained and calibrated.[1,29]

The NMOC data are to be collected during the season of peak ozone concentrations (summer). Because NMOC concentrations are apt to be relatively high in central urban locations at those times of the day (early morning) when

these measurements are required for use in EKMA more confidence can be placed in the estimate. Data from a recent study of continuous NMOC instruments suggest that relative standard deviations of 30 percent are likely for well operated and maintained instruments when concentrations are above 0.5 - 1.0 ppmC. However, because of the uncertainties in individual NMOC readings, the NMOC/NO_x ratio calculated at a single site for a single day is not recommended for use in city-specific EKMA. Considering FID instrument reliability and model sensitivity, the following procedure is recommended for calculating NMOC/NO_x ratios.

Recommended Procedure:

1. Individual NMOC/NO_x ratios at a site are calculated as the ratio of the 6-9 a.m. LCT average NMOC and NO_x concentrations, i.e., the average of the hourly concentrations for hours 6-7, 7-8, and 8-9 LCT, respectively. Ratios should not be calculated for any day with less than two valid hours for either NMOC or NO_x.

2. If precursor measurements from more than one urban site are available for the same day as the ozone design value, and the individual ratios at each site do not differ by more than 30 percent from the average ratio, then the design ratio (DR) is the average of the individual 6-9 a.m. NMOC/NO_x ratios. If data from only one site are available for a specific day, the design ratio for that day should be calculated using the procedure described in (3) below.

$$DR = \frac{\sum_{i=1}^{n} (R_i)}{n} = \bar{R}$$

where

R_i = 6-9 a.m. (NMOC/NO_x) ratio at Site i

$\bar{R}$ = the average ratio

n = the number of sites

3. If only one site measuring both NMOC and NO_x is available, or if the values from different sites are missing or not comparable (i.e., some ratios differ by more than 30% from the mean ratio), the following procedure is recommended. The ratio for use with the isopleth diagram should be calculated as the median of the ratios observed on all those days being modeled with accompanying NMOC and NO_x data.

$$DR = \text{median } \{R_j\}, \text{ for a single site}$$

or

$$DR = \text{median } \{\overline{R}_j\}, \text{ for multiple sites}$$

where

j = a high ozone day, and $j = 1,2,\ldots,N$

When the monitor is located in a relatively high and uniform emission density area, good agreement has been found between ratios calculated on individual high ozone days and more robust measures.[1,2,18] Thus, use of the median ratio is viewed as providing a robust estimate of the daily design ratio which is consistent with the conceptual basis of the model.

4. If no collocated pairs of NMOC and NO_x monitors were operated in the urban area during one or two of the years in the suggested three year period, it is recommended that the procedure in (3) above be followed using the available NMOC/NO_x data to choose a median NMOC/NO_x ratio. In this case, the median ratio would be used with ozone data from all years without the appropriate precursor concentration data.

Two examples of calculating NMOC/NO_x ratios for use with EKMA/OZIPP are contained in Figure 3-6.

3.3 USE OF OZIPP TO GENERATE ISOPLETH DIAGRAMS

An ozone isopleth diagram is to be generated for each day investigated. Section 3.1 described the procedures for deriving the day-specific modeling data, and Section 3.2 described the formulation of the empirical data. This section briefly addresses the procedures for producing a day-specific diagram using these data. The details are described in Reference 3, the OZIPP User's Manual.

The modeling data are input to OZIPP by means of option cards. Table 3-3 shows the appropriate option card to be used with each category of model variables described in Section 3.1. There are only two other important considerations. First, the diagram must contain the starting point defined by the intersection of the design NMOC/NO_x ratio and the daily design ozone level. This is accomplished by selecting appropriate NMOC and NO_x scales on the abscissa and ordinate,

Example 1.

Given: Ratios at five urban core sites on the day being modeled are respectively 9.1, 6.2, 6.4, 6.5 and 9.8

Find: The NMOC/NO_x ratio for use in EKMA

Solution: First calculate the average ratio

$$\overline{R} = \frac{9.1 + 6.2 + 6.4 + 6.5 + 9.8}{5}$$

$$\overline{R} = 7.6$$

Note that all the ratios are within $\pm$ 30% of $\overline{R}$, i.e., all the ratios are between 5.3 and 9.9. Then, the design ratio is

$$DR = \overline{R} = 7.6$$

Example 2.

Given: Assume that only one site is available for the study. Assume also that the NMOC/NO_x ratios are available for five of the design days. These ratios are 8.8, 8.6, 15.5, 9.7, and 14.3, respectively.

Find: The design ratio for use with all the design days.

Solution: Since only one site is available, the design ratio is

$$DR = \text{median } (8.8, 8.6, 15.5, 9.7, 14.3)$$

$$DR = 9.7$$

FIGURE 3-6. Example Calculations of the Design NMOC/NO_x Ratio

Table 3-3. OZIPP Options For Model Input Data

Input Data	Section	OZIPP Option
Light Intensity	3.1.1	PLACE
Dilution	3.1.2	DILUTION
O_3 Transport	3.1.3	TRANSPORT
Precursor Transport	3.1.4	TRANSPORT
Post-8:00 a.m. Emissions	3.1.5	EMISSIONS
Reactivity	3.1.6	REACTIVITY*

* Since OZIPP default values are recommended, this option may be omitted.

respectively. Reference 3 provides guidance for choosing the proper scales using the ISOPLETH option. Secondly, isopleths corresponding to the ozone daily design value and to 0.12 ppm should be incorporated in the diagram to facilitate control calculations. This is also accomplished by using the ISOPLETH option. Consequently, a day-specific isopleth diagram can be generated by proper specification of the ISOPLETH option in addition to those listed in Table 3-3.

4.0 CALCULATION OF CONTROL ESTIMATES

The previous Chapter described procedures for deriving day-specific ozone isopleth diagrams. These diagrams are used to calculate VOC emission controls necessary to reduce the peak ozone level observed at a particular site on an individual day to 0.12 ppm. The SIP requirement is determined from those results according to the method described in Section 2.3. This Chapter describes the techniques that are used to calculate the VOC emission reduction estimates for each site-day in order to determine the SIP control requirement.

In estimating the degree of VOC control necessary to reduce peak ozone levels to 0.12 ppm, the role of NO_x should be accounted for. This is accomplished by estimating the change in NO_x between the base period and the future period which is of interest. For the 1982 SIPs, the most straight-forward procedure for estimating this change is to project the expected percent change in total region-wide NO_x emissions between the base period and 1987. Factors to consider include growth, anticipated effects of various control programs, and technological advancements.

The first step in calculating controls using a diagram is to establish a starting point on the diagram. This point is defined by the intersection of the design NMOC/NO_x ratio line with the isopleth corresponding to the ozone daily design value, and represents the base case conditions (i.e., base emissions, base transport, etc.). All other points on the diagram represent the effects of changing precursor emissions relative to the base case assuming that everything else remains constant. Thus, control requirements may be calculated for a given day using a single diagram if:

1) Initial precursor concentrations and post 8:00 a.m. emissions are reduced proportionally, and

2) All other non-emission factors (e.g., transported ozone) remain constant.

A second situation arises if there is a concurrent change in emissions and some other factor, or if post 8:00 a.m. emissions are not reduced proportionally with initial concentrations. However, meteorological conditions must be assumed to be the same in the future case as in the base case, e.g., mixing heights will be the same for both diagrams. In this case, two isopleth diagrams are required: (1) a diagram applicable for base case conditions, and (2) a diagram applicable for the future (i.e., the post-control period in 1987), which reflects the concurrent changes described above. This situation is discussed in Section 4.2.

4.1 USE OF SINGLE DAY-SPECIFIC DIAGRAMS

An isopleth diagram derived for a specific day corresponds to the base period. If non-emission conditions corresponding to the base period are expected to remain unchanged, then the single day-specific diagram can be used to estimate the VOC control requirements. The single diagram cannot be used if one of the following situations is expected to occur between the base period and the future period of interest (e.g., 1987):

1) ozone transported into the area changes

2) precursors transported into the area change

3) the diurnal emission pattern changes grossly (i.e., hourly emissions change independently of one another).

If one or more of these situations is anticipated, the procedures described in Section 4.2 must be followed.

The procedure for arriving at the necessary VOC emission reduction is outlined in Table 4-1 and an example is shown in Figure 4-1. The starting point on the diagram is located by the intersection of the design NMOC/NO_x ratio line with the isopleth corresponding to the daily ozone design value. The NMOC and NO_x coordinates of this point correspond to the base case conditions to which all changes in NO_x and/or NMOC must be referenced. The next step is to estimate the change in NO_x between the base state and the future period. The base NO_x level is adjusted by the percent change in total NO_x emissions anticipated between the two periods. A post-control point is then located on the 0.12 ppm isopleth at the point reflecting the projected change in NO_x. The final step in the calculation is to compute the percent change in NMOC required to reduce NMOC from the base point to the post-control point. This percent reduction is the degree of VOC emission control necessary to reduce the peak ozone level to 0.12 ppm.

4.2 CONCURRENT CHANGES IN EMISSIONS AND OTHER FACTORS

Consideration of different control measures that are implemented concurrently necessitates using a different procedure than that described in Section 4.1. The major examples of concurrent implementation of control measures include:

1) reduction in local precursors and reduction of ozone transported into a city;

2) reduction in local precursors and reduction of precursors transported into a city;

Table 4-1. Control Calculations Using A Single Isopleth Diagram

Step 1: Locate the base-case point on the diagram by finding the intersection of the design NMOC/NO_x ratio line with the isopleth for the ozone daily design value. Let the NMOC and NO_x coordinates of this point be signified by $(NMOC)_1$ and $(NO_x)_1$, respectively.

Step 2: Calculate the post-control NO_x coordinate by adjusting the base NO_x level by the expected percent change in NO_x emissions between the base and post-control periods. Let the post-control NO_x coordinate be signified by $(NO_x)_2$. Thus,

$$(NO_x)_2 = (NO_x)_1 \times (1 + \frac{\Delta NO_x}{100})$$

where

$(NO_x)_2$ = post-control NO_x coordinate

$(NO_x)_1$ = base case NO_x coordinate

ΔNO_x = expected change in NO_x, percent

Step 3: Locate the post-control point on the diagram by finding the post-control NO_x coordinate, $(NO_x)_2$, on the 0.12 ppm ozone isopleth. Let the NMOC coordinate of this point be $(NMOC)_2$.

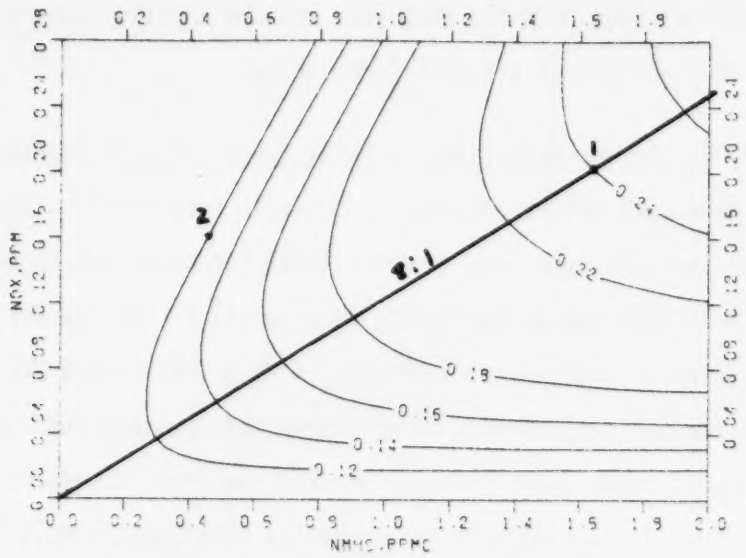
Step 4: Compute the percent reduction necessary to lower $(NMOC)_1$ to $(NMOC)_2$. Thus,

$$\% \text{ Reduction in VOC} = [1 - \frac{(NMOC)_2}{(NMOC)_1}] \times 100$$

GIVEN: O_3 Daily Design Value = .24
Design NMOC/NO_x = 8:1
Anticipated Change in NO_x = -20%
Base case diagram shown below

FIND: Percent reduction in VOC emissions needed to reduce ozone from .24 to 0.12 ppm

SOLUTION:



BASE CASE DIAGRAM: O3 PLOT = .12

STEP 1: The base case point is found by the intersection of the 8:1 NMOC/NO_x ratio line with the .24 ozone isopleth (Point 1) on the diagram. At Point 1, $(NMOC)_1 = 1.64$ and $(NO_x)_1 = .205$

STEP 2: The post-control NO_x coordinate is calcualted as follows:

$$(NO_x)_2 = (.205) \times (1 - \frac{20}{100}) = .164$$

STEP 3: The post-control point is located at the intersection of the .164 NO_x coordinate and the 0.12 ppm ozone isopleth (Point 2). At Point 2, $(NMOC)_2 = 0.46$

STEP 4: The VOC emission reduction is calculated as

$$\% \text{ reduction} = (1 - \frac{.46}{1.64}) \times 100 = 72\%$$

Figure 4-1. Example emission reduction calculation using a single ozone isopleth diagram

3) reduction in local precursors and gross changes in diurnal emission patterns;

4) combinations of the above.

In each case, the procedure for calculating VOC emission reductions requires the development of an additional isopleth diagram. The VOC emission reduction is then calculated using both the base case and the additional diagram. Each of the above four situations are considered below.

4.2.1 Concurrent Reductions in Local Precursors and Transported Ozone

When calculating emission reductions, consideration should ordinarily be given to the situation when future transported ozone concentrations may be different from the base period levels as a result of the imposition of control measures upwind of the city of interest. Before calculating VOC emission reductions, an isopleth diagram must be generated for the post-control case, i.e., the case in which the ozone transported into the area is reduced. It must be recognized that it is difficult to generalize about what should be assumed concerning future levels of transported ozone. One source of this difficulty arises as a result of the differing characteristics of "upwind areas." For example, in the Northeastern United States, one could expect greater reductions in "future transported ozone" than in many other areas. The greater reductions would occur because of large designated nonattainment areas for ozone which are upwind of northeastern cities. Nonattainment areas are subject, at a minimum, to emission controls arising from the Federal Motor Vehicle Control Program (FMVCP), application of Best Available Control Technology (BACT) on new sources of VOC, phasing out of old, poorly controlled stationary sources and application of Reasonable Available Control Technology (RACT) on existing sources. In many

other areas of the country however, upwind areas are predominantly unclassified or attainment areas. These areas are subject only to the FMVCP and emission reduction which might occur as the result of existing, poorly controlled sources being retired and replaced with new sources having BACT. The procedures described below require case by case judgments as to whether areas upwind of a city being modeled are primarily nonattainment areas or otherwise. Once this judgment is made, these procedures may be used to estimate the degree of reduction expected due to control programs implemented upwind of the city. Following this discussion is a description of the quantitative techniques for estimating VOC emission reductions.

A. Estimating Future Transport of Ozone

Recall from Section 3.1.3 that ozone may be transported in both the surface layer and aloft. As was described in that section, several studies have shown that advection of ozone aloft appears to be the more significant mechanism of transport from one area to another. If control programs are implemented in upwind areas, ozone transported into the city is likely to be reduced. However, in most cases, the source area and the level of future controls are not likely to be known to any degree of certainty.

Recommended Procedure: Because of the considerable uncertainty in the location and future control levels of the source area(s) for ozone transported into the urban area, the relationship depicted in Figure 4-2 is recommended for estimating the future ozone transport level given the level of present transport. The solid curve in Figure 4-2 was derived on the basis of changes in VOC emissions which are projected assuming a national mix of source categories; national estimates of projected growth in stationary source emissions and vehicle miles traveled (VMT); anticipated impact of applying reasonably available control technology (RACT) to stationary sources and the impact of the Federal Motor Vehicle Control Program on mobile sources; and consideration of natural background levels.[2,32-35] It was assumed that future ozone levels would not exceed the NAAQS. The solid curve is most appropriate for use by cities subject to impacts from large upwind nonattainment areas. The dashed curve in Figure 4-2

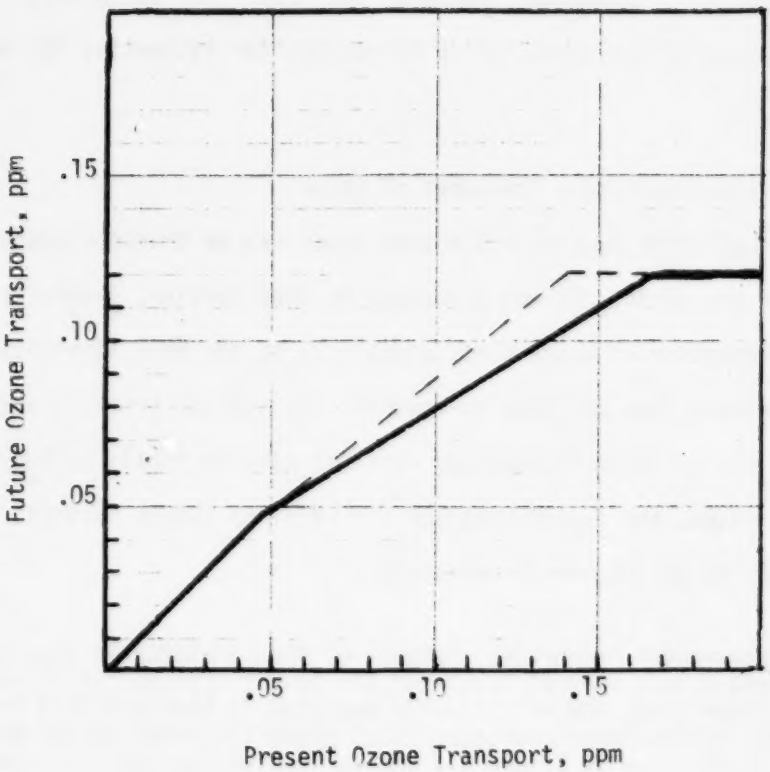


Figure 4-2 Future Ozone Transport as a Function of Present Transport

differs from the solid curve only in that the impact of RACT is ignored. The dashed curve is most appropriate for use when a city is isolated and not impacted by large designated nonattainment areas.

Without information to the contrary, future transport along the surface should be assumed equal to zero. If significant non-zero concentrations were found for present ozone transport along the surface, then future ozone transport levels should be obtained using the relationships shown in Figure 4-2.

B. Calculation of VOC Emission Reductions

The computational procedure for determining the required VOC emission reductions is outlined in Table 4-2, and an example problem is shown in Figure 4-3. The procedure is similar to that described in Section 4.1. The starting point for the calculation is found in exactly the same manner as described in Section 4.1, i.e., by the intersection of the design NMOC/NO_x ratio line and the ozone isopleth corresponding to daily ozone design value on the base case diagram. Again, the NMOC and NO_x coordinates of this point correspond to the base case conditions to which any changes in NMOC and/or NO_x must be referenced. The post-control point is found exactly as was previously described, except that a diagram corresponding to future transported ozone level is used. Changes expected in NO_x are first calculated by adjusting the base NO_x level (i.e., the NO_x coordinate of the starting point) by the assumed percent change in NO_x expected between the base period and the post-control period. The post-control point is found on the 0.12 ppm isopleth of the future case diagram at the post-control NO_x level. The NMOC reduction is then determined by calculating the percent reduction necessary to reduce NMOC from the base point to the post-control point. This percent reduction is the VOC emission reduction necessary to reduce the peak ozone concentration to 0.12 ppm, assuming that ozone transported aloft changes in the future.

Table 4-2. Control Calculations Using Two Isopleth Diagrams

Step 1: After developing a base case diagram, generate a future-case diagram for the post-control period. For example, if transported ozone is expected to be reduced, a diagram reflecting that reduction should be generated.

Step 2: Locate the base-case point on the base-case diagram by finding the intersection of the design NMOC/NO_x ratio line with the isopleth for the ozone daily design value. Let the NMOC and NO_x coordinates of this point be signified by $(NMOC)_1$ and $(NO_x)_1$, respectively.

Step 3: Calculate the post-control NO_x coordinate by adjusting the base NO_x level by the expected percent change in NO_x emissions between the base and post-control periods. Let the post-control NO_x coordinate be signified by the $(NO_x)_2$. Thus,

$$(NO_x)_2 = (NO_x)_1 \times (1 + \frac{\Delta NO_x}{100})$$

where

$(NO_x)_2$ = post-control NO_x coordinate

$(NO_x)_1$ = base case NO_x coordinate

ΔNO_x = expected change in NO_x, percent

Step 4: Locate the post-control point on the future-case diagram by finding the post-control NO_x coordinate, $(NO_x)_2$, on the 0.12 ppm ozone isopleth. Let the NMOC coordinate of this point be $(NMOC)_2$.

Step 5: Compute the percent reduction necessary to lower $(NMOC)_1$ to $(NMOC)_2$. Thus,

$$\% \text{ Reduction in VOC} = [1 - \frac{(NMOC)_2}{(NMOC)_1}] \times 100$$

GIVEN: O_3 Design Value = .24

Design NMOC/NO_x = 8:1

Present Transport of O_3 Aloft = .12

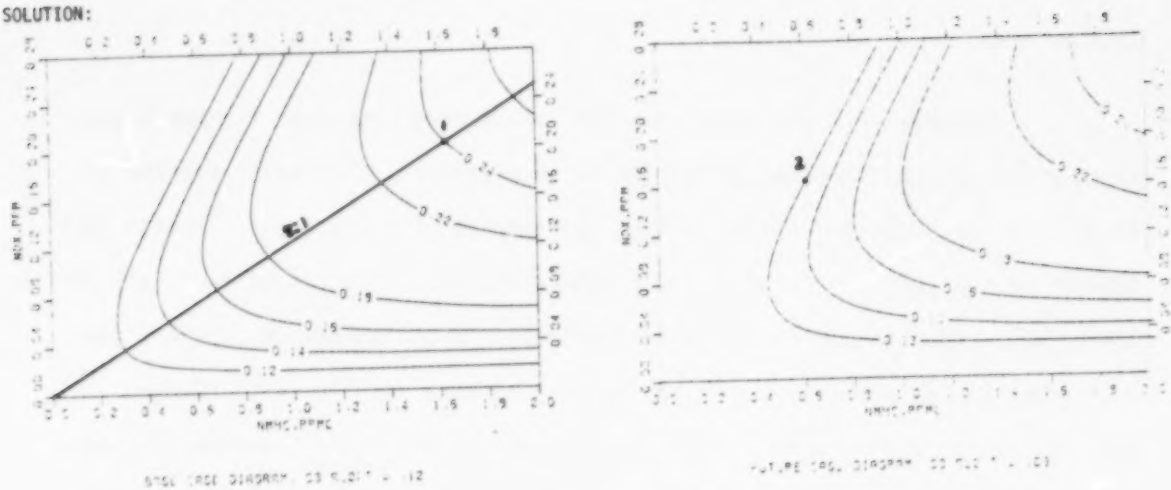
Future Transport of O_3 Aloft = .09 (from Figure 4-2)

Anticipated change in NO_x = -20%

Base case and future diagrams shown below.

FIND: Percent reduction in VOC needed to reduce ozone from .24 to .12 ppm

SOLUTION:



STEP 1: The future case diagram shown above was generated by using the OZIPP input data for the base case diagram, except that ozone transported aloft was changed from 0.12 to 0.09 ppm.

STEP 2: The base case point is found by the intersection of the 8:1 NMOC/NO_x ratio line with the .24 ozone isopleth (Point 1) on the base case diagram. At Point 1, $(NMOC)_1$ = 1.64 and $(NO_x)_1$ = .205

STEP 3: The post-control NO_x coordinate is calculated as follows:

$$(NO_x)_2 = (.205) \times (1 - \frac{20}{100}) = .164$$

STEP 4: The post-control point is located on the future case diagram at the intersection of the .164 NO_x coordinate and the 0.12 ppm ozone isopleth (Point 2). At Point 2 $(NMOC)_2$ = .61

STEP 5: The VOC emission reduction is calculated as:

$$\% \text{ reduction} = (1 - \frac{.61}{1.64}) = 63\%$$

Figure 4-3. Example emission reduction calculation considering changes in transported ozone.

4.2.2 Concurrent Reductions in Local Precursors and Transported Precursors

As was described in Section 3.1.4, the transport of precursors is not considered essential in most instances, especially if upwind reductions parallel local reductions. However, if precursor transport is deemed critical, procedures that may be employed are addressed in detail in Appendix B. The conceptual framework for considering precursor transport is discussed below, along with procedures for estimating changes in future levels of precursors transported into an area.

Conceptually, the procedures for considering precursor transport are exactly the same as those described for ozone transport. The major problem is estimating the precursor concentrations transported into the area. This in part depends on the geographical location of the city, and is addressed in detail in Appendix B. Because control programs are likely to be implemented upwind, the concentrations of precursors transported into an area are likely to change. Described below are procedures that may be used to estimate the changes in precursor levels transported into an area. These may be applied to both surface layer transport and transport aloft where applicable.

Recommended Procedure: Because of the considerable uncertainty in future control levels for the source area(s) for precursors transported into an urban area, the following reductions are recommended: NMOC transported concentrations may be reduced up to 40% in cities being impacted by upwind nonattainment areas and up to 20% in other cities. NO_x levels are not projected to change significantly, so no change should be assumed. The basis for these recommendations is the projection of VOC and NO_x emissions that was described in Section 4.2.1 on estimating future transported ozone levels.

Alternate Procedure: If specific information concerning the primary source of precursors transported into the urban area, and the scheduled controls for that area are available, then estimates of future transport may be developed using a proportional model. However, the source area should be clearly identified through the use of trajectory analysis and the assumptions concerning the implementation of future controls should be fully documented.

The procedures for considering precursor transport aloft are exactly the same as those described for ozone transport. A base case diagram is used in conjunction with a diagram representing the post-control state. The first represents the base case with existing transported levels, while the second diagram corresponds to the situation in which changes in precursor transport are expected. The procedures outlined in Table 4-2 are also applicable to this case. The procedure for considering precursor transport in the surface layer is more complex, and is discussed in Appendix B.

4.2.3 Concurrent Changes in Local Precursors and Diurnal Emission Patterns

Gross changes in the diurnal emission pattern expected between the base period and the post-control period can be incorporated into an analysis. It must be emphasized that these changes must be significant and on a scale as large as, or larger than, the spatial and temporal resolution of the emissions inventory used in the analysis (see Section 3.1.5). Because of the assumptions inherent in the model, evaluation of small scale changes cannot be made using EKMA. Thus, for example, the OZIPP/EKMA approach could not be used to evaluate the effects of constructing a new highway. However, it could be used to assess the effects of large scale changes, such as a suburban county substantially increasing emissions relative to an urban county as a result of rapid growth.

The procedures for incorporating changes in diurnal emission patterns are similar to those for treating changes in transported pollutants. A base case diagram is developed using the existing emission information, and a diagram representative of future emissions is developed incorporating the expected changes in the diurnal emission pattern. The expected changes must be derived from locally applicable projections. For example, an increase in emissions in one or

more counties might be anticipated due to population growth or industrial expansion. This expected increase would be incorporated in the analysis by developing a future case diagram using the emission fractions corresponding to the projected emissions increase. Thus, if a two-fold increase in county-wide emissions (in the absence of controls) is assumed for a county, the emission fractions for the affected county would be doubled for generating the future case diagram. Control calculations are performed exactly in the manner described in Table 4-2.

Normally, consideration of changes in diurnal emission patterns will not be necessary. The modeler will have to decide whether or not any anticipated changes are significant enough to warrant special consideration.

4.2.4 Consideration of Multiple Changes

The previous three sections summarized the procedures for calculating control estimates for cases in which local precursors are reduced and one other significant change is expected to occur. If more than one additional change is anticipated, the same procedures can be used. In addition to the base case diagram, one diagram reflecting all future changes is developed. For example, assume transported ozone, transported precursors, and gross changes in the diurnal emission pattern are all expected. The base case diagram would be developed using the base case transported ozone, transported precursors, and diurnal emission fractions. The second diagram would be developed using the future transported ozone levels, future transported precursor levels, and the emission fractions corresponding to the projected diurnal emission pattern. This new diagram would incorporate all changes simultaneously, and any calculated VOC emission reductions would reflect these assumptions. However, the future case diagram would still use the same meteorological conditions, e.g., parcel path and

mixing heights, as the base case. The calculations themselves would be carried out just as outlined in Table 4-2.

5.0 ACKNOWLEDGEMENT

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APPENDIX A

ESTIMATION OF MIXING HEIGHTS FOR USE IN OZIPP

In OZIPP, the rate of dilution of atmospheric pollutants is governed by the diurnal change in mixing height. The mixing height is the top of a surface-based layer of air which is well-mixed due to mechanical and thermal turbulence. As described in Section 3.1.2, the input variables required for OZIPP include: the mixing height at 0800 LCT, the maximum mixing height, the time at which the mixing height begins to rise if it starts to rise after 0800 LCT, and the time at which the mixing height reaches its maximum. The rate of rise is computed internally by OZIPP.

Three different procedures for determining daily morning and afternoon mixing heights were outlined in Section 3.1.2. The recommended procedure entails the use of temperature soundings taken routinely by the National Weather Service at various locations throughout the United States. If more direct measurements are available (e.g., radiosondes taken in the urban area or sodar data), they may be used instead of NWS data. If neither of the above two sets of measurements can be used, then the use of 250 m for the 0800 LCT mixing height and the climatological mean value for the maximum mixing height is recommended. The procedures to be followed for each approach are described below.

A.1 RECOMMENDED PROCEDURE USING NWS RADIOSONDES

Temperature soundings are taken by the NWS at sites throughout the United States. Soundings are usually taken every 12 hours at 1200 and 0000 Greenwich Mean Time (GMT), corresponding to 0800 and 2000 Eastern Daylight Time, respectively. Therefore, to estimate daily mixing heights, (1) a NWS site must be selected which is representative of the city of interest, (2) appropriate sounding data and urban surface data must be obtained, and (3) these data must be used to compute the morning and maximum mixing heights. Each of these steps is discussed below.

A.1.1 Site Selection

In selecting a NWS site as the basis for mixing height estimation, care should be taken to insure that the site is meteorologically representative of the city of interest. Table A-1 contains recommended sites for a number of cities. Backup sites are listed for those cases in which radiosonde data may not be available for a given day, or if the site has significantly different meteorological conditions. Examples of the latter are the case in which a surface front lies between the sounding site and the city or the city is clear but cloudiness or precipitation occurs at the sounding site.

A.1.2 Selection of Day Specific Data

The daily morning mixing height for the model is normally estimated using the 1200 GMT (0800 EDT) sounding, while the maximum mixing height is estimated using the 0000 GMT (2000 EDT) sounding. In some cases, these soundings may not be available or appropriate and alternate approaches will be necessary. Table A-2 summarizes the order of preference in selecting the radiosondes for estimating the daily mixing heights. The actual data may be obtained from the National Climatic Center (NCC).*

In addition to the sounding data, surface temperature and pressure data are also needed for each day modeled. The urban surface temperature at 0800 LCT (or the average temperature between 0800-0900 LCT) and the maximum

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*National Climatic Center, Federal Building, Asheville, NC 28801
Telephone: (704) 258-2850, x203
Please allow about four weeks for NCC to fill an order.

Table A-1.

City	NWS Radiosonde Stations		Climatological Mixing Heights (m AGL)
	PRIMARY	BACKUP(S)	MAX
Allentown, PA	NYC, NY; Atl City, NJ	Albany, NY; Dulles AP, VA	1825
Baltimore, MD	Dulles AP, VA	Wallops Is., VA; Atl City, NJ	1825
Boston, MA	Portland, ME	Albany, NY; Chatham, MA	1375
Bridgeport, CT	NYC, NY; Atl City, NJ	Albany, NY	1500
Chicago, IL/IN	Peoria, IL	Green Bay, WI	1575
Cincinnati, OH/KY	Dayton, OH	Huntington, WV	1650
Cleveland, OH	Dayton, OH	Buffalo, NY	1650
Dayton, OH	*Dayton, OH	Huntington, WV	1661
Denver, CO	*Denver, CO	Grand Junction, CO	3358
Detroit, MI	Flint, MI	Dayton, OH	1700
Fresno, CA	Oakland, CA	Vandenberg AFB, CA	2000
Hartford, CT	Albany, NY	NYC, NY; Atl City, NJ	1500
Houston, TX	Victoria, TX	Lake Charles, LA	1525
Indianapolis, IN	Dayton, OH	Peoria, IL; Salem, IL	1600
Los Angeles, CA	Vandenberg AFB, CA	San Diego, CA	603
Louisville, KY/IN	Dayton, OH	Nashville, TN	1700
Milwaukee, WI	Green Bay, WI	Peoria, IL	1575
Nashville, TN	*Nashville, TN	Jackson, AL	1845
New Haven, CT	NYC, NY; Atl City, NJ	Albany, NY	1450
New York, NY/NJ	*NYC, NY; Atl City, NJ	Albany, NY	1512
Philadelphia, PA/NJ	NYC, NY; Atl City, NJ	Dulles AP, VA	1700
Phoenix, AZ	Tucson, AZ	Winslow, AZ;	3250
Pittsburgh, PA	*Pittsburgh, PA	Dayton, OH; Dulles AP, VA	1794
Portland, OR	Salem, OR	Medford, OR; Quilayute, WA	1575
Providence, RI	New York, NY	Albany, NY; Chatham, MA; Atl City, NJ	1350
Richmond, VA	Dulles AP, VA	Greensboro, NC; Wallops Is., VA	1725
Sacramento, CA	Oakland, CA	Vandenberg AFB, CA	1600
St. Louis, MO/IL	Salem, IL	Peoria, IL; Monett, MO	1625
Salt Lake City, UT	*Salt Lake City, UT	Grand Junction, CO	3673
San Bernardino, CA	San Diego, CA	Vandenberg AFB, CA	1200
San Diego, CA	*San Diego, CA	Vandenberg AFB, CA	564
San Fransciso, CA	Oakland, CA	Vandenberg AFB, CA	625
Scranton, PA	NYC, NY; Atl City, NJ	Albany, NY; Atl City, NJ Dulles AP, VA	1850
Seattle, WA	Quilayute, WA	Salem, OR	1398
Springfield, MA	Albany, NY	NYC, NY; Atl City, NJ	1600
Trenton, NJ	NYC, NY; Atl City, NJ	Dulles AP, VA	1700
Ventura-Oxnard, CA	Vandenberg AFB, CA	San Diego, CA	610
Washington DC/MD/VA	*Dulles AP, VA	Wallops Is., VA	1884
Wilmington, DE	Dulles AP, VA; Atl City, NJ	Wallops Is., VA; New York, NY	1700
Worcester, MA	Albany, NY	Portland, ME; Chatham, MA	1500
Youngstown, OH	Pittsburgh, PA	Buffalo, NY; Dayton, OH	1700

* This station should be used unless the data is missing for all the times listed in Table A-2. However, if a frontal passage occurs between the time of maximum ozone and the time of the launch of the 0000 GMT sounding (normally about 2300 GMT), the 1200 GMT sounding from that site should be used.

NOTE: The NYC, NY radiosonde station was replaced by Atlantic City, NJ on September 2, 1980.

Table A-2. Preferential Order of Data Selection

Morning Mixing Height Estimate

1. 1200 GMT Sounding at Primary Site
2. 0600 GMT Sounding at Primary Site*
3. 1200 GMT Sounding at Backup Site
4. 0600 GMT Sounding at Backup Site*

Maximum Mixing Height Estimate

1. 0000 GMT Sounding at Primary Site
2. 1800 GMT Sounding at Primary Site*
3. 1200 GMT Sounding at Primary Site
4. 0000 GMT Sounding at Backup Site
5. 1800 GMT Sounding at Backup Site*
6. 1200 GMT Sounding at Backup Site

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* Soundings are not normally taken at these times, but may be available in some instances.

temperature occurring prior to 1800 LCT are needed to estimate the morning and maximum mixing height, respectively. The surface temperature data should be measured to the nearest 0.1°C at a well ventilated site. The site should be located near the center of the urban area. Surface atmospheric pressure measurements are needed at the same time and location of the urban surface temperature measurements, if at all possible. If these measurements are not available, a local NWS or Federal Aviation Administration weather reporting station's barometer reading may be used.

If the elevation of the pressure reading and the urban temperature site are different, an adjustment should be made to the pressure measurement using equation (3).

$$P_{sfc} = P_{obs} + [.11mb/m \times (Z_{obs} - Z_{sfc})] \quad (3)$$

where

Z_{obs} = the elevation, in meters above sea level (mASL), of the pressure measurement

Z_{sfc} = the elevation (mASL) of the urban temperature measurement

P_{obs} = the pressure, in millibars, at Z_{obs}

P_{sfc} = the pressure, in millibars, at the urban temperature site

NOTE: Z_{obs} will be equal to zero meters ASL when a pressure reduced to sea level is used.

The value of P_{sfc} from equation (3) is an approximate value and can be rounded to the nearest whole millibar.

A.1.3 Mixing Height Estimation

The procedures for estimating the 0800 LCT mixing height and the maximum mixing height are outlined in Table A-3. These procedures have been automated. Appropriate computer listings and a User's Guide can be obtained from the authors. The procedures in Table A-3 are designed for use with the worksheet displayed in Table A-4. Figure A-1 contains a flow diagram of the process. The procedures use the mandatory and significant pressure levels reported for each sounding (Table A-5). The steps lead to determination of the height at which the adiabatic lapse rate (extended from the surface temperature and pressure) intersects the vertical temperature profile. (For background information, the reader is referred to References 21, 36-37.) An example problem is presented in Section A.4.

In some instances, the mixing heights estimated by this procedure may not be representative. If the 0800 LCT morning mixing height is estimated to be less than 250 meters, then a value of 250 meters should be used. This assumed minimum value for the 0800 LCT mixing height accounts for the effects of mixing due to mechanical turbulence caused by increased surface roughness in the urban area.[11,38] Similarly, if the city's maximum mixing height is greater than twice the climatological maximum value (e.g., see Table A-1), the surface temperature and pressure used and the choice of sounding site should be checked for representativeness using the guidelines in A.1.1 and A.1.2 above. If no backup data are available, twice the climatological value should be used as the maximum. Also, a maximum mixing height less than or equal to the morning mixing height, or less than one-third the climatological maximum mixing height value is suspect. Using data from a backup site may provide a more realistic value. However, if

Table A-3. Procedures for Estimating Mixing Heights

Step 1 -- For reference, the information at the top of Table A-4 should be listed (e.g., date, city, etc.). If the morning mixing height is to be calculated, the 0800 LCT surface data are used. If the maximum mixing height is to be calculated, the data corresponding to the time of maximum temperature (i.e., between 800-1800 LCT) are used. In the row labeled URBAN SURFACE DATA, enter the following information: 1) the elevation of the urban temperature site in meters above sea level; 2) the surface pressure in millibars (this value is P_{sfc}); and 3) the surface temperature in degrees Celsus (°C).

Convert the surface temperature in column four to degrees Kelvin (°K) by adding 273.2, and enter the result in column five. This value is T_{sfc}(°K).

Use Equation 1 below and the values just entered to calculate the potential temperature at the surface (θ_{sfc} in °K to the nearest 0.1°K) and enter this value under column six "θ(°K)".

$$\theta_{sfc} \text{ (in °K)} = T_{sfc} \text{ (in °K)} \left(\frac{P_{sfc} \text{ (in mb)}}{1000 \text{ mb}} \right)^{-0.286} \qquad (1)$$

Step 2 -- Using the temperature sounding data, find the highest pressure level other than the sounding's surface value that is less than the pressure at the urban surface.* From this pressure level on the sounding, enter the height (if listed), pressure and temperature (in °C) into the row marked "(2)" on Table A-4.

Step 3 -- Convert the temperature at this level to the Kelvin scale and enter in column 5. Compute the potential temperature (θ_p) to the nearest 0.1°K using the pressure (P, in mb) and temperature (T_p in °K) at this level in Equation 2 below:

$$\theta_p \text{ (in °K)} = T_p \text{ (in °K)} \left(\frac{P \text{ (in mb)}}{1000 \text{ mb}} \right)^{-0.286} \qquad (2)$$

Enter the value of θ_p found from Equation (2) into the same row under the column labeled "θ(°K)".

Step 4 -- If the potential temperature, "θ," of the last row that was entered is greater than the potential temperature θ_{sfc}, and this is the first level above the surface, then 250 meters should be used as the mixing height. Otherwise, go to Step 5. If it is less than or equal to θ_{sfc}, then enter the height (if given), pressure and temperature of the next lowest pressure level found on the sounding into the next row of Table A-4 and return to Step 3.

Step 5 -- The mixing height is between the last two levels entered into Table A-4. If height values are given for both of these levels, the elevation of the mixing height can be found using Step 6. If one of the levels does not have a height value, use linear interpolation to find the pressure value for the potential temperature value of θ_{sfc} + 0.1°K. Enter this pressure value into the row marked "MIXING HEIGHT" at the bottom of Table A-4 under the column "PRESSURE in mb." Proceed to Step 7.

Step 6 -- From the two levels where height is given on the sounding surrounding the mixing height level, use linear interpolation to find the height (in meters ASL) at the value θ_{sfc} + 0.1°K (i.e., the potential temperature θ at the mixing height). Enter the value found by linear interpolation into the row labeled "MIXING HEIGHT" under the column "HEIGHT (mASL)" and proceed to Step 8.

Step 7 -- Use linear interpolation to find the height above sea level of the mixing height using the pressure at the mixing height (found in Step 5) and the pressure levels on the sounding above and below the mixing height pressure that have both pressure and height values. Enter the height value found into the row "MIXING HEIGHT" under the column marked "HEIGHT, (mASL)" and proceed to Step 8.

Step 8 -- Subtract the elevation of the urban site (mASL) from the height (mASL) of the mixing height. The result is the height of the mixing height in meters above the surface of the city (mAGL). Enter this value into Table A-4.

NOTE; Despite the fact that pressure and height, and potential temperature and height, are not linearly related, linear interpolation does not produce significant errors over the limited ranges used above.

* For example, if the urban surface pressure is 965 mb, and the sounding pressures are: 1005, 1000, 963, 850 mb, etc., 963 mb is the "highest pressure level that is less than the pressure at the urban surface." 850 mb is the "next lowest pressure level" needed in Step 4.

Table A-4. Worksheet for Computing Mixing Heights

Date: Time Of Mixing Height For Input Into Model:

City: Sounding Method:

Time of Sounding: LCT. Surface elevation: mASL

Location of Sounding:

LOCATION OF URBAN SURFACE DATA (IF DIFFERENT THAN ABOVE) -

1	2	3	4	5	6	7
LEVEL	HEIGHT (mASL)	PRESSURE (mb)	TEMP. (°C)	TEMP. (°K)	Θ (°K)	REMARKS
Urban Surface Data (1)						$\leftarrow \Theta_{sfc}$
(2)						

	Θ_{sfc} + 0.1°K (°K)	PRESSURE (mb)	HEIGHT (mASL)	HEIGHT (mAGL)	HEIGHT USED IN MODEL (mAGL)
MIXING HEIGHT					

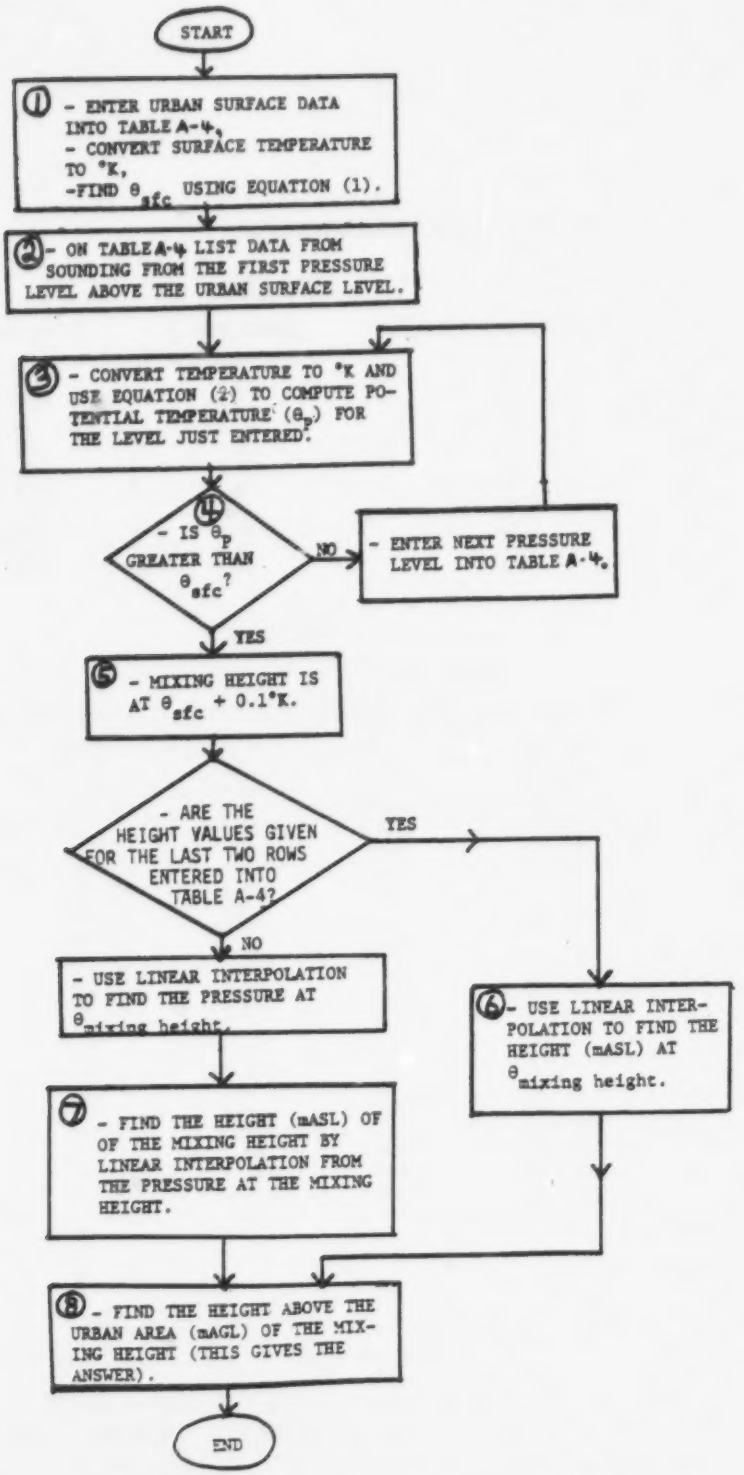

START
① - ENTER URBAN SURFACE DATA INTO TABLE A-4,
- CONVERT SURFACE TEMPERATURE TO °K,
-FIND θ_{sfc} USING EQUATION (1).
② - ON TABLE A-4 LIST DATA FROM SOUNDING FROM THE FIRST PRESSURE LEVEL ABOVE THE URBAN SURFACE LEVEL.
③ - CONVERT TEMPERATURE TO °K AND USE EQUATION (2) TO COMPUTE POTENTIAL TEMPERATURE (θ_p) FOR THE LEVEL JUST ENTERED.
④ - IS θ_p GREATER THAN θ_{sfc}?
NO
- ENTER NEXT PRESSURE LEVEL INTO TABLE A-4.
YES
⑤ - MIXING HEIGHT IS AT θ_{sfc} + 0.1°K.
- ARE THE HEIGHT VALUES GIVEN FOR THE LAST TWO ROWS ENTERED INTO TABLE A-4?
YES
NO
- USE LINEAR INTERPOLATION TO FIND THE PRESSURE AT $\theta_{mixing\ height}$.
⑥ - USE LINEAR INTERPOLATION TO FIND THE HEIGHT (mASL) AT $\theta_{mixing\ height}$.
⑦ - FIND THE HEIGHT (mASL) OF OF THE MIXING HEIGHT BY LINEAR INTERPOLATION FROM THE PRESSURE AT THE MIXING HEIGHT.
⑧ - FIND THE HEIGHT ABOVE THE URBAN AREA (mAGL) OF THE MIXING HEIGHT (THIS GIVES THE ANSWER).
END

Figure A-1. Flow Chart for Table A-3. Numbers in circles are step numbers in Table A-3.

Table A-5. Surface and Sounding Data

Surface Data

Hour Starting at, LCT	Temperature °C	Pressure, mb
8	23.2	1010.3
9	23.9	1010.7
10	25.8	1010.8
11	27.3	1010.6
12	28.7	1010.3
13	29.3	1010.0
14	30.1	1009.6
15	30.4	1009.2
16	30.8	1008.8
17	31.4	1008.6
18	31.2	1008.5

Sounding Data

1200 GMT Sounding			0000 GMT Sounding		
Pressure (mb)	Height (m ASL)	Temp. (°C)	Pressure (mb)	Height (m ASL)	Temp. (°C)
S 1015	8*	23.0	S 1012	8*	31.0
M 1000	139	23.0	M 1000	114	30.6
S 967	---	24.4	M 850	1537	16.4
M 850	1550	16.2	S 831	---	15.4
S 827	---	14.2	S 791	---	13.2
S 817	---	13.6	S 778	---	11.8
M 700	3168	4.6	S 760	---	11.2
S 680	---	5.6	M 700	3164	7.0
S 661	---	5.6	S 628	---	1.6
S 608	---	0.4	S 560	---	-1.5
M 500	5860	-8.3	M 500	5860	-7.3
S 491	---	-9.3	M 400	7560	-18.9
S 453	---	-12.7	S 371	---	-21.7
S 438	---	-13.9	M 300	9650	-33.1
M 400	7560	-18.7	S 265	---	-39.9
S 388	---	-20.1	M 250	10900	-42.9
S 349	---	-26.3	S 205	---	-52.9
S 324	---	-29.7	M 200	12370	-53.3
M 300	9640	-33.7	M 150	14190	-61.1
S 267	---	-39.5	S 127	---	-64.9
M 250	10890	-47.7	S 120	---	-61.7
M 200	12370	-51.7	M 100	16690	-63.3
M 150	14190	-60.9	M 70	18900	-58.5
S 148	---	-61.5	M 50	21040	-54.5
			M 30	24350	-49.9
			M 20	27030	-44.7
			S 15	---	-42.1

Note: M = Mandatory Levels and S = Significant Levels

If NWS Data are used, both the mandatory and significant levels are needed.

The 0000 GMT Sounding is the following day in GMT.

* The lowest level of the sounding should not be used in the mixing height calculations.

the low afternoon mixing height is due to the existence of a surface-based stable layer, an adjustment to the procedures outlined in Table A-3 can be employed. Replace the "Urban Surface Data" with the following data from the sounding site: 1) the maximum temperature, 2) the estimated or observed surface pressure at the time of maximum temperature, and 3) the height of the sounding surface level. Then compute the mixing height according to the procedure in Table A-3. If this problem occurs on a majority of modeling days, then an alternative, more representative site should be used for all the modeling days.

A.2 USE OF ALTERNATE DATA

Other, more direct measurements of mixing height may be used to increase the representativeness of the estimated values. These methods include direct urban temperature sounding and sodar data. The measurements should be taken over the urban area near the center of the city at 0800 LCT, and close to the time of the climatological maximum surface temperature. It is not recommended that these measurements be taken specifically for the OZIPP/EKMA techniques; however, they may be employed if available. Examples are discussed below.

1) Local Urban Radiosonde -- the methods described in Section A.1.3 can be used to find the mixing height from radiosondes taken within the urban area as opposed to NWS sites. The radiosonde surface temperature and pressure should be used in place of the URBAN SURFACE DATA.

2) Urban Helicopter Soundings -- Similarly, vertical temperature profiles obtained from helicopter soundings can be used in place of the NWS soundings. The urban site surface temperature and pressure should be used as the URBAN SURFACE DATA.

3) Sodar -- (also known as Acoustic Radar) the mixing height found by sodar (in mAGL) can be used directly in the model.

NOTE: Regardless of the procedure applied, the limitations concerning the morning and maximum mixing heights that were described in Section A.1.3 should be observed.

A.3 USE OF CLIMATOLOGICAL MEANS

If radiosonde data are not available, 250 m should be used for the 0800 LCT mixing height and the city-specific climatological mean value may be used for the maximum mixing height. Table A-1 lists representative values for several cities, and Reference 12 contains information for the contiguous United States. If Reference 12 is used, values for summer, non-precipitation days should be used. The appropriate starting and ending times of the mixing height rise in the model are 0800 LCT and the time of the maximum temperature. If the latter is unknown, 1400 LST (1500 LDT) may be assumed.

A.4 EXAMPLE PROBLEM

To illustrate the procedure described in Section A.1.3, an example problem is included for reference. Table A-5 shows relevant data typically available. Note that both the 1200 GMT and the 0000 GMT soundings are used in the calculations, the former for the morning mixing height and the latter for the maximum mixing height. Table A-6 shows the individual computational steps for the morning mixing height calculation, while Table A-7 shows the same for the maximum mixing height.

Table A-6. Morning Mixing Height Determination --

Example from Table A-5:

08 LCT Temperature = 23.2°C

Maximum Temperature after 08 LCT = 31.4°C at 17 LCT

08 LCT Pressure = 1010.3 mb

Pressure at time of maximum temperature (1700 LCT) = 1008.6 mb

Time of morning mixing height = 0800 LCT

Time of maximum mixing height = 1700 LCT

Problem:

Find the 0800 LCT mixing height using data from the sounding shown in Table A-5 (i.e., the 1200 GMT sounding). A worksheet is shown as Table A-6A. The elevation of the urban surface site is 62 mASL.

Solution:

STEP 1

Enter 62., 1010.3 and 23.2 into row (1) of Table A-6A (URBAN SURFACE DATA)

TEMP (°C) = 23.2

Converted to °K = 23.2 + 273.2 = 296.4°K

Enter 296.4 into row (1) of Table A-6A under "TEMP(°K)"

Using Equation (1) on the Urban Surface Data:

$$\theta_{sfc} = 296.4°K \left(\frac{1010.3 \text{ mb}}{1000. \text{ mb}}\right)^{-0.286}$$

$$\theta_{sfc} = 295.5°K$$

STEP 2 - Enter 139., 1000. and 23.0 into row (2) of Table A-6A.

STEP 3 - 23.0 + 273.2 = 296.2°K

Using Equation (2):

$$\theta_p = 296.2°K \left(\frac{1000 \text{ mb}}{1000 \text{ mb}}\right)^{-0.286}$$

θ_p = 296.2°K (Enter this value into Table A-6A)

STEP 4 - θ_p (296.2°K) is greater than θ_{sfc} (295.5°K).

Since θ_p is from the first level above the surface, the 250 m default value should be used for the 0800 LCT mixing height.

Table Example (Hypothetical Data)

Date: DATE OF MODELING Time of Mixing Height For Input Into Model: 0800 EDT

City: CITY TO BE MODELED Sounding Method: NWS, URBAN RADIOSONDE OR HELICOPTER

Time of Sounding: 0800 LCT. Surface Elevation: (OF SOUNDING) mASL

Location of Sounding: NAME OF SOUNDING SITE

LOCATION OF URBAN SURFACE DATA (IF DIFFERENT THAN ABOVE) - STREET ADDRESS, BUILDING OR PARK, ETC.

1	2	3	4	5	6	7
LEVEL	HEIGHT (mASL)	PRESSURE (mb)	TEMP. (°C)	TEMP. (°K)	θ (°K)	REMARKS
Urban Surface Data (1)	62	1010.3	23.2	296.4	295.5	← θ_{sfc}
(2)	139	1000.	23.0	296.2	296.2	θ AT THIS LEVEL IS HIGHER THAN θ_{SFC} + 0.1 °K.

	θ_{sfc} + 0.1°K (°K)	PRESSURE (mb)	HEIGHT (mASL)	HEIGHT (mAGL)	HEIGHT USED IN MODEL (mAGL)
MIXING HEIGHT	295.6	—	0	0	250

Table A-7. Maximum Mixing Height Determination

Example from Table A-5:

08 LCT Temperature = 23.2°C

Maximum Temperature = 31.4°C at 17 LCT

08 LCT Pressure = 1010.3 mb

17 LCT Pressure = 1008.6 mb

Time of morning mixing height = 0800 LCT

Time of maximum mixing height = 1700 LCT

Problem:

Find the maximum afternoon mixing height using data from the sounding shown in Table A-5 (i.e., the 0000 GMT sounding). A worksheet is shown as Table A-7A. The elevation of the urban site is 62 mASL.

Solution:

STEP 1 -

Enter 62, 1008.6 and 31.4 into row (1) of Table A-7A (Urban Surface Data)

TEMP (°C) = 31.4°C

Converted to °K = 31.4 + 273.2 = 304.6°K

Enter 304.6°K into row (1) of Table A-7A under "TEMP (°K)

Using Equation (1) on the Urban Surface Data

$$\theta_{sfc} = 304.6°K \left(\frac{1008.6\ mb}{1000\ \ mb}\right)^{-0.286}$$

$$\theta_{sfc} = 303.9$$

STEP 2 -

Enter 114., 1000., and 30.6 into Table A-7A.

STEP 3 -

30.6°C + 273.2 = 303.8°K

Using Equation (2):

$$\theta_p = 303.8°K \left(\frac{1000\ mb}{1000\ mb}\right)^{-0.286}$$

$$\theta_p = 303.8°K$$

STEP 4 - 303.8°K is less than 303.9°K
Therefore, enter 1537., 850. and 16.4 into Table A-7A.
and return to STEP 3.

STEP 3 - 16.4°C + 273.2 = 289.6°K

Using Equation (2)

$$\theta_p = 289.6°K \left(\frac{850\ \ mb}{1000\ mb}\right)^{-0.286}$$

$$\theta_p = 303.4°K$$

STEP 4 - 303.4°K is less than 303.9°K
Therefore, enter 831. and 15.4 into Table A-7A (note that there is no height value for this pressure level) and return to STEP 3.

Table A-7 (Continued)

STEP 3 - 15.4°C + 273.2 = 288.6°K

Using Equation (2):

$$\theta_p = 288.6°K \left(\frac{831\ mb}{1000\ mb}\right)^{-0.286}$$

$$\theta_p = 304.3°K$$

STEP 4 - 304.3°K is greater than 303.9°K

STEP 5 -

$$\theta_{sfc} + 0.1°K = 303.9°K + 0.1°K = 304.0°K$$

Using linear interpolation from potential temperature (θ) to pressure since a highest value is not given for the 831 mb pressure level

θ (°K)	Pressure (mb)
303.4	850
304.0	P mixing height
304.3	831

$$\text{P mixing height} = 831\ mb - \frac{(850\ mb - 831\ mb)(304.0°K - 304.3°K)}{304.3°K - 303.4°K}$$

$$= 831 - \frac{(19\ mb)(-0.3°K)}{0.9°K}$$

$$= 837.3\ mb$$

The pressure at the mixing height (rounded to the nearest whole millibar) is 837 mb.

STEP 7 -

Use linear interpolation to find the height above sea level of the mixing height. Enter 3164. and 700. into Table A-7A.

PRESSURE (mb)	HEIGHT (mASL)
850	1537.
837	Z mixing height
700	3164.

$$\text{Z mixing height} = 1537\ m + \frac{(3164\ m - 1537\ m)(837\ mb - 850\ mb)}{700\ mb - 850\ mb}$$

$$= 1537\ m + \frac{(1627\ m)(-13\ mb)}{-150\ mb}$$

Z mixing height = 1678 m

STEP 8 -

1678 mASL - Height of mixing height
- 62 mASL - Elevation of urban surface site
1616 mAGL = Mixing height in meters above the urban area.

1616 m is the height of the maximum mixing height to be used in the model with the time of 1700 LCT.

Table Example (Hypothetical Data)

Date: Time of Mixing Height For Input Into Model: 1700 EDT

City: Sounding Method: NWS.

Time of Sounding: 2000 LCT. Surface Elevation: 8. mASL

Location of Sounding:

LOCATION OF URBAN SURFACE DATA (IF DIFFERENT THAN ABOVE) -

1	2	3	4	5	6	7
LEVEL	HEIGHT (mASL)	PRESSURE (mb)	TEMP. (°C)	TEMP. (°K)	θ (°K)	REMARKS
Urban Surface Data (1)	62	1008.6	31.4	304.6	303.9	← θ_{sfc}
(2)	114	1000.	30.6	303.8	303.8	
	1537	850.	16.4	289.6	303.4	MIXING HEIGHT IS BETWEEN THESE TWO LEVELS AT θ = 304.0°K
	—	831.	15.4	288.6	304.3	
	3164	700.	—	—	—	NEEDED TO PROVIDE UPPER HEIGHT VALUE FOR INTERPOLATION.

	θ_{sfc} + 0.1°K (°K)	PRESSURE (mb)	HEIGHT (mASL)	HEIGHT (mAGL)	HEIGHT USED IN MODEL (mAGL)
MIXING HEIGHT	304.0	837.	1678.	1616.	1616.

APPENDIX B

CONSIDERATION OF PRECURSOR TRANSPORT

Transport of pervasive, high precursor concentrations into a city as a result of emissions from upwind sources presents difficulties in applying city-specific EKMA. One difficulty is estimating the concentrations of precursors transported into the urban area. Such estimates generally require special monitoring programs to detect transported pollutant levels. Often, data may not be available for a specific day being investigated. This is further complicated by the fact that transported pollutant concentrations are strongly affected by the meteorological conditions on a given day, making any generalizations regarding treatment of transport difficult. In spite of these difficulties, general quantitative techniques have been developed to account explicitly for the role of precursor transport. As will be described, some sensitivity analyses have been performed using these techniques. The results indicate that consideration of precursor transport is not normally necessary, and is not recommended. However, the techniques are presented for those cases in which explicit treatment of precursors is perceived by a user as an important consideration in the overall modeling analysis.

Three topics are discussed below: 1) the transport of precursors aloft; 2) the transport of precursors in the surface layer; and 3) the case in which the nonattainment area consists of more than one high-emission density area.

B.1 PRECURSOR TRANSPORT ALOFT

Most evidence suggests that concentrations of precursors transported aloft are usually very low.[13,14,17,18] Generally, concentrations of NMOC measured above the morning mixing height have been found to be less than 0.1 ppmC. NO_x levels transported from upwind areas above the morning mixed layer are usually much less than concentrations attributable to the urban area. Table B-1 summarizes

Table B-1. Typical Effects of NMOC Transport Aloft on Control Estimates*

O_3 Design Value	NMOC/NO_x	Base Case NMOC Transported Aloft, ppm .05	.10	.15
.18	8:1	+4	+8	+12
.18	12:1	+3	+5	+8
.18	16:1	+1	+3	+4
.24	8:1	+3	+5	+8
.24	12:1	+2	+4	+7
.24	16:1	+3	+5	+7
.30	8:1	+2	+3	+5
.30	12:1	+2	+4	+5
.30	16:1	+2	+3	+4

* Entries in the table represent the typical difference between considering precursor transport aloft versus neglecting its effect. For example, if the control estimate obtained by considering transported NMOC were 50%, and that computed using the normal OZIPP/EKMA technique (i.e., neglecting transport) were 45%, a difference of 5% in control level would be recorded in the table.

the results of a sensitivity analysis that was performed to assess the effects of considering NMOC transport. These tests were conducted using conditions likely to be associated with what is believed to be unusually high concentrations of precursor transport. Since areas experiencing significant precursor transport would likely be subject to relatively high ozone concentrations transported aloft, the concentration of ozone transported aloft was assumed equal to 0.12 ppm. However, control estimates were made assuming that both ozone and precursors transported aloft would be reduced according to the recommended approach described in Sections 4.2.2 and 4.2.3. The table shows the difference in control estimates obtained by explicit consideration of precursor transport aloft versus using the OZIPP/EKMA technique in the normal manner. For example, if the control estimate obtained by considering precursor transport explicitly were 50%, and that obtained using the normal method were 45%, the difference of +5% would be reported in the table. The results reveal that differences in control estimates are small for concentrations of NMOC transported aloft which are less than about 0.1 ppmC. As a result of these findings, and the uncertainties and difficulties associated with measuring precursors aloft, explicit consideration of precursor transport aloft is <u>not</u> normally recommended. If, however, conditions are such that explicit treatment is perceived by the user as essential, the required additional measurements and the manner in which these measurements can be employed in an OZIPP/EKMA application are described below.

The only appropriate method for estimating precursor concentrations aloft is by direct measurement, such as airborne measurements or those taken on tall towers. Surface measurements of precursors may not be good indications of precursor transport aloft because of possible influences of surface layer

transport and local generation. Thus, precursor transport aloft can only be considered if direct measurements are available. These measurements should be made in the early morning, upwind of the city, at a height above the morning mixed layer but below the anticipated maximum daily mixing height. Enough samples should be taken to insure that five measurements are available on days for which precursor transport is likely to be important (i.e., on which the prevailing wind flow may be from highly industrialized or urbanized areas upwind and conditions are conducive to ozone formation). Normally, this requires a five to six week sampling program. Reference 13 contains guidance on obtaining direct measurements.

Explicit Consideration of Precursors Transported Aloft: If direct measurements of precursors aloft are available on the day being investigated, they may be used directly in the modeling analysis. If no measurements were taken on the day being modeled, but are available for days with somewhat similar meteorological conditions (e.g., wind is from the same general direction), then the median value of these measurements may be used. At least five measurements taken on days conducive to high ozone formation are necessary for estimating the median value. In either of the above cases, care should be taken to insure that the measurements used are truly representative of the vertical concentration profile above the mixed layer. For example, a measurement of high concentration above the mixed layer may reflect the presence of a plume within that layer, but may not be representative of concentrations extending throughout the layer found above the mixed layer. Figure B-1 illustrates the problem.

The quantitative treatment of precursors transported aloft is analogous to that of ozone transported aloft (see Section 4.2.1). A base case diagram is first developed with the precursor concentrations transported aloft estimated according to the procedure described in the preceding paragraph. A post-control diagram is then generated using precursor concentrations aloft which reflect the effects of upwind control programs. Section 4.2.2 describes the methodologies for estimating future concentrations of precursors transported aloft. The computational procedures necessary to estimate the necessary VOC reductions are also described in Section 4.2.2, and summarized in Table 4-2.

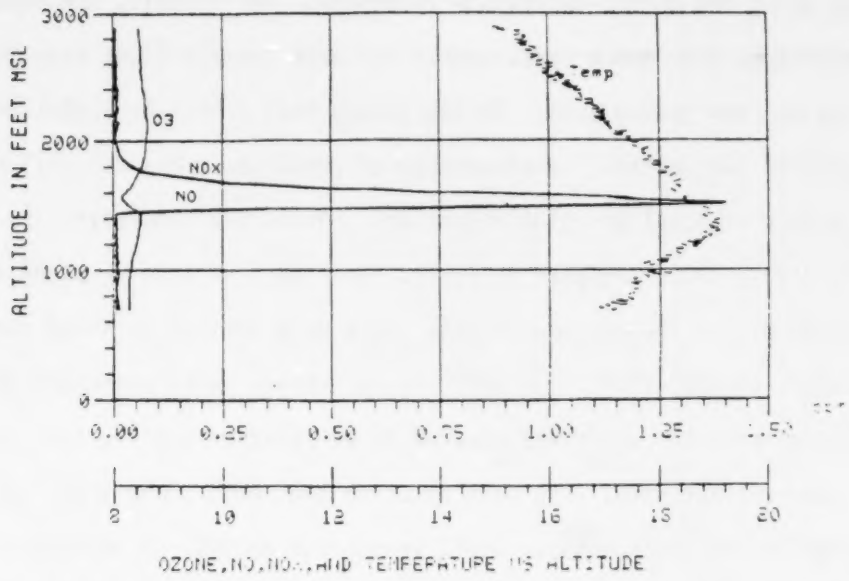


Figure B-1. Vertical Pollutant Profile Illustrating a Shallow Layer of Elevated NO_x Concentrations Aloft.

B.2 PRECURSOR TRANSPORT IN THE SURFACE LAYER

Similar to transport of precursors aloft, most evidence suggests that urban concentrations resulting from precursors being transported within the surface layer are usually negligible.[13,14,17,18] Furthermore, the contribution of precursors transported in the surface layer to urban levels is accounted for to some degree by using the normal OZIPP/EKMA technique. For example, the design NMOC/NO_x ratio determined from urban measurements reflects contributions from both the urban area and the upwind area. To the extent that precursor reductions in both areas parallel one another, consideration of precursor transport will have little, if any, effect on local emission reductions. Table B-2 summarizes the results of some sensitivity tests designed to assess the effect of incorporating the transport of NMOC within the surface. These tests were similar to those conducted for the transport of NMOC aloft. In addition to surface layer transport of NMOC, the concentration of ozone aloft was assumed to be relatively high, i.e., 0.12 ppm. However, control estimates were made assuming that both ozone aloft and precursors transported in the surface layer would be reduced by 40%, as described in Sections 4.2.2 and 4.2.3. The table shows the difference in control estimates obtained by explicitly considering surface layer transport versus using the OZIPP/EKMA in the normal manner (i.e., surface layer transport is not explicitly considered). The differences are generally small, especially for contributions from upwind areas less than 30%. Thus, because of the insensitivity, and because of the approximations and assumptions that must be made in order to evaluate surface layer transport explicitly, consideration of precursor transport within the surface layer is <u>not</u> generally recommended. However, if consideration of precursor transport is perceived as a critical issue in the modeling analysis, the additional measurements which are necessary and the manner in which they are

Table B-2. Typical Effects of NMOC Surface Layer Transport on Control Estimates*

O_3 Design Value	$NMOC/NO_x$	Contribution of Surface Transport to Urban Levels, percent** 5-10	10-20	20-30	30-40
.18	8:1	+1	+2	+3	+3
.18	12:1	+2	+1	+2	+3
.18	16:1	+1	+1	+1	+2
.24	8:1	+3	+1	+1	-3
.24	12:1	+2	+3	+4	+4
.24	16:1	+2	+4	+5	+8
.30	8:1	+1	+1	0	+1
.30	12:1	+2	+2	+3	+6
.30	16:1	+2	+2	+4	+7

* Entries in the table represent the typical difference between considering NMOC transport in the surface layer versus neglecting its effect. For example, if the control estimate obtained by considering transported NMOC were 50%, and the estimate derived using the normal OZIPP/EKMA technique (i.e., neglecting transport) were 45%, a difference of +5% would be entered in the table.

** A 10% contribution implies that 90% of the urban, 6-9 a.m. concentration is due to local generation and 10% is due to transport from upwind.

used in the analysis are described below.

The determination of surface layer transport is accomplished by means of surface based measurements taken at the upwind edge of an urban area. It is recognized, however, that upwind measurements will not always be available for the days of interest. The technique described below makes use of the available upwind measurements. References 13 and 29 contain guidance on monitor siting and sampling. However, deployment of a continuous NMOC analyzer for the sole purpose of estimating precursor transport is not recommended. Rather, collection of a limited number of discrete samples, analyzed chromatographically with the species summed to yield total NMOC, is preferable for estimating upwind NMOC. These upwind samples should be collected between 6-9 a.m. LCT. In order to adequately characterize precursor transport, samples for a minimum of five days on which meteorological conditions favor significant transport (i.e., days on which the prevailing wind flow may be from highly industrialized on urbanized areas upwind and conditions are conducive to ozone formation) should be available. Normally, a five to six week sampling program will be adequate.

Explicit Treatment of Surface Layer Transport: Table B-3 summarizes the computational procedures for considering surface layer transport of precursors. The concepts employed to account for surface layer transport are 1) to estimate the contribution of transported precursors to urban levels using available upwind measurements and corresponding urban area measurements, and 2) to incorporate these relative contributions in the OZIPP/EKMA technique. The first two steps involve estimating typical relative contribution of precursor transport to urban levels. Thus, for example, a median contribution factor of .5 implies that 50% of the precursor concentrations measured in the urban area are due to precursor transport. Contribution factors should be computed separately for NMOC and/or NO_x. Steps 3 through 5 entail quantifying precursor transport relative to the normal OZIPP/EKMA base case point. The precursor concentration to be entered in OZIPP as surface layer transport is calculated in Step 4, and the design NMOC/NO_x ratio is adjusted to remove the relative contribution of precursor transport (Step 5). In Step 6, a new base case diagram is generated to reflect the effects of precursor transport in the surface layer. As indicated in Step 7, the estimation of future transport, development of a post-control diagram, and subsequent

Table B-3. Explicit Treatment of Surface Layer Precursor Transport

1. Compute the ratio of upwind measurements to urban average levels for each day on which upwind measurements are available.

$$(CF)_i = \frac{(C_{upwind})_i}{(C_{urban})_i}$$

where

$(CF)_i$ = fractional contribution of transported levels to urban levels for day i

$(C_{upwind})_i$ = upwind 6-9 a.m. precursor measurement for day i

$(C_{urban})_i$ = 6-9 a.m. urban average concentration (if data from more than one monitor are available, the 6-9 levels for each monitor are averaged).

2. Determine the typical transport level by taking the median of the contribution factors calculated in Step 1. Let this factor be represented by $\widetilde{CF}$.

3. Generate a base case isopleth diagram neglecting the contribution of surface layer transport. Determine the base case point by finding the intersection of the design NMOC/NO_x ratio with the isopleth corresponding to the daily design value. Let the coordinates of this point be represented by $(NMOC)_1$ and $(NO_x)_1$. (Note that this is identical to what is done when precursor transport is not considered.)

4. Estimate the relative contributions of transported precursors by multiplying the contribution factor(s) by the corresponding base coordinate(s) found in Step 3. Thus,

$$(C_{TRAN})_{NMOC} = (\widetilde{CF})_{NMOC} \times (NMOC)_1$$

$$(C_{TRAN})_{NO_x} = (\widetilde{CF})_{NO_x} \times (NO_x)_1$$

where

C_{TRAN} = Relative Transported Concentration

$(\widetilde{CF})$ = Contribution Factor calculated in Step 2

$(NMOC)_1$, $(NO_x)_1$ = Base case coordinates found in Step 3

5. Compute an adjusted NMOC/NO_x ratio to remove the contribution of transported precursors.

$$R_{adj} = \frac{[1-(\widetilde{CF})_{NMOC}]}{[1-(\widetilde{CF})_{NO_x}]} R$$

where

R = normal NMOC/NO_x ratio calculated according to Section 3.2.2

R_{adj} = an NMOC/NO_x ratio adjusted to remove the contribution of transported

6. Develop a new base case diagram. The relative precursor concentrations calculated in Step 4 are entered in the OZIPP model as the concentrations of precursors transported in the surface layer. [If post 8 a.m. emissions are considered, the emission fractions calculated according to Section 3.1.5 must also be divided by $1.-(\widetilde{CF})$.]

7. Follow the procedures described in Section 4.2.2 for calculating VOC emission reductions. The diagram developed in Step 6 serves as the base case diagram, and the adjusted NMOC/NO_x ratio calculated in Step 5 should be used as the design ratio.

GIVEN: O_3 Design Value = .24

Design $NMOC/NO_x$ = 8:1

Present Transport of O_3 Aloft = .12

Future Transport of O_3 Aloft = .09

Anticipated change in NO_x = -20%

Median contribution factor for NMOC = .25

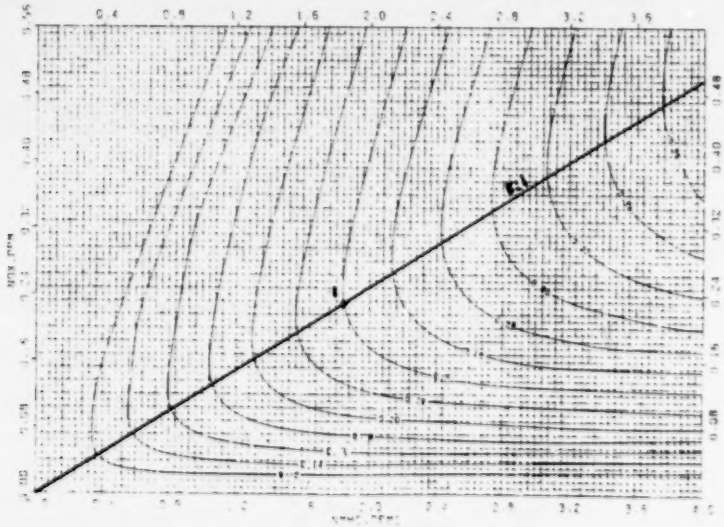
Median contribution factor for NO_x = 0.0

FIND: Percent reduction in VOC needed to reduce ozone from .24 to 0.12 ppm, assuming that future surface transport of NMOC will be reduced by 40%.

SOLUTION:

STEPS 1 and 2: The median contribution factors are 0.25 for NMOC and 0.0 for NO_x. Therefore, only the transport of NMOC will be considered.

STEP 3: The base case diagram (neglecting transport) is shown below. The base case point is found in the normal fashion, i.e., the intersection of the .24 isopleth with the 8:1 $NMOC/NO_x$. The coordinates of this point are $(NMOC)_1 = 1.85$ and $(NO_x)_1 = .231$



STEP 4: The relative contribution of NMOC transported in the surface layer is calculated as follows:

$$(C_{TRAN})_{NMOC} = (.25) \times 1.85 = .46$$

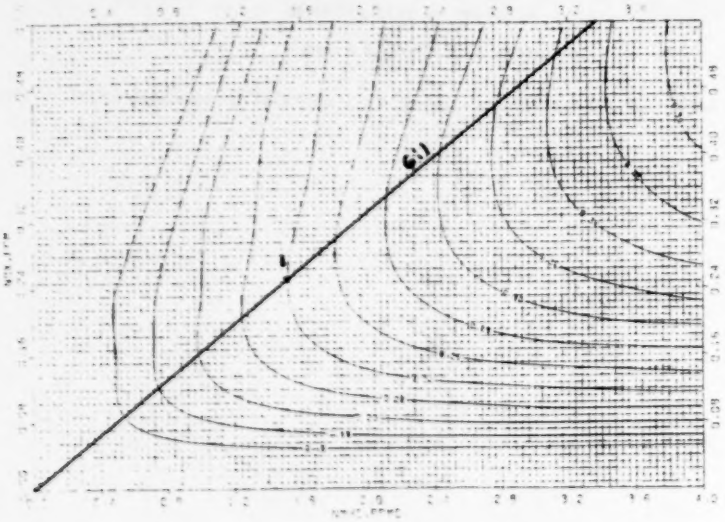
$$(C_{TRAN})_{NO_x} = 0.0$$

STEP 5: The adjusted $NMOC/NO_x$ ratio is computed as follows:

$$R_{ADJ} = \frac{(1.-0.25)}{(1.-0.0)} \times 8.0 = 6.0$$

Figure B-2. Example emission reduction calculation with the explicit consideration of precursor transport in the surface layer.

STEP 6: The new base case diagram is shown below. The following modifications were made to the input data that was used to generate the original base diagram (Step 3): 1) surface layer NMOC transport was set to .46 as opposed to zero for the original diagram; and 2) the emission fractions for NMOC were each divided by 1.0 - .25 = .75.



The starting point (Point 1) on this diagram is found by finding the intersection of the adjusted $NMOC/NO_x$ ratio line (6:1 in this case) with the .24 ozone isopleth. The coordinates of this point are $(NMOC)_1 = 1.52$ and $(NO_x)_1 = .253$.

STEP 7: A future case diagram is developed to reflect the expected changes in transported pollutants. Thus, the input data used to generate the base diagram (Step 6) is modified as follows: 1) ozone transported aloft is set to .09 rather than .12 (see Section 4.2.2); and 2) NMOC transported in the surface layer is reduced from .46 to .28 (see Section 4.2.3). The resultant diagram is shown below.

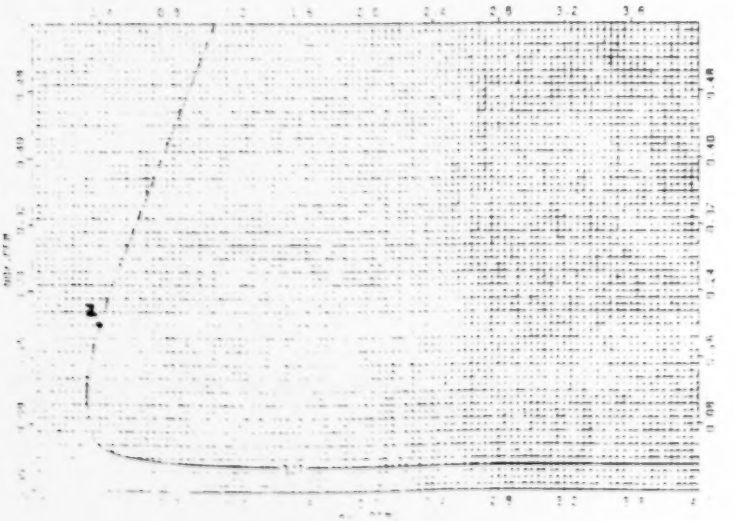


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Figure B-2. Example emission reduction calculation with the explicit consideration of precursor transport in the surface layer. (continued)

The post-control point is found in the normal fashion. First, the post-control NO_x point is calculated:

$$(NO_x)_2 = (.253) \times (1 - \frac{20}{100}) = .202$$

The post-control point is then located on the future case diagram at the inter-section of the .202 NO_x coordinate and the 0.12 ppm ozone isopleth (Point 2). At Point 2, $(NMOC)_2 = .40$. The VOC emission reduction is calcualted as

$$\% \text{ reduction} = (1 - \frac{.40}{1.52}) = 74\%$$

Note that the base point used in this calculation was that found in Step 6, not that in Step 3.

Figure B-2. Example emission reduction calculation with the explicit consideration of precursor transport in the surface layer. (continued)

calculation of the VOC emission reduction is carried out according to the procedure described in Section 4.2.2. An example is presented in Figure B-2.

The above procedure represents an idealized situation, so extreme care should be taken in its application. First, the procedure should only be applied to days with similar meteorological conditions (i.e., the wind is out of same general direction). Second, only days with meteorological conditions conducive to high ozone formation should be considered. Third, siting of upwind monitors is critical. Any upwind measurements that are affected by local sources will invalidate the approach. Also, the upwind measurements must be taken close enough to the urban area so that further significant dilution of the tranported precursor concentrations does not occur. Consequently, the approach can only be used for contribution factors less than one. A contribution factor greater than one indicates the assumptions underlying the approach have been violated, and the normal OZIPP/EKMA application (i.e., precursor transport is not explicitly incorporated) must be employed.

B.3 MORE THAN ONE HIGH EMISSION DENSITY AREA

In some instances, more than one high emission density area may be found within the region for which a control program(s) is being developed. Examples include the following:

1) An urban core and a second separate, clearly defined industralized area with high emission density;

2) One urbanized area located in two different States, for which a separate control program must be devloped for each area due to jurisdictional considerations;

3) Urbanized areas which consist of two separate, clearly defined, urban cores (e.g., twin cities).

Such geographies may present special problems in applying the OZIPP/EKMA technique.

Ideally, the OZIPP/EKMA technique should be applied in exactly the same manner as described in Chapter 3, i.e., the column should be assumed to originate in the urban core and move directly towards the site of peak ozone concentration. The urban core should always be used as the origin of column movement because the chemical kinetic mechanism is based upon reactions of NMOC/NO_x mixtures representative of automotive exhaust. Surface wind measurements should be analyzed to insure that the peak ozone level is located in the general downwind direction of the urban core of interest. However, an exact trajectory cannot usually be determined due to uncertainties in deriving the spatial and temporal variations in wind fields. Consequently, some assumptions in estimating trajectories must be made.

First, consider the case of an industrialized area located near an urban area. In most instances, the routine OZIPP/EKMA application will provide the best estimate of overall regional control targets. However, in some cases the industrial area may be quite removed from the urban core. If the two areas are separated by a region of little or no source activity, the procedures outlined in the previous subsection on precursor transport could be employed in those instances on which the industrial area contributes to the urban area (i.e., the urban area is downwind of the industrial region). However, estimates of control of the industrial area must be arrived at independently of the OZIPP/EKMA technique. Using the industrial area as the origin for the column movement would be inappropriate considering the chemistry is more representative of automotive exhaust mixtures.

For the case in which an urban area is divided by a jurisdictional boundary (e.g., a State), the ideal method is to develop one control estimate for the entire urban area (i.e., treat the urban area as one entity). If this cannot be done because of jurisdictional considerations, each area should be treated as an entity, and the same procedure followed for each area. Figure B-3 illustrates the types of assumptions that could be made for trajectories under two different situations.

The case of two separate urban cores in a region may be treated in one of three ways. An independent analysis could be performed for each urban core. Alternatively, the major city could be chosen as the design case, and the results of that analysis applied to each city. A third alternative is to use the procedures described in B.2 of this appendix when appropriate. However, for this procedure to be applicable, the cities must be separated by a region of little or no precursor source activity.

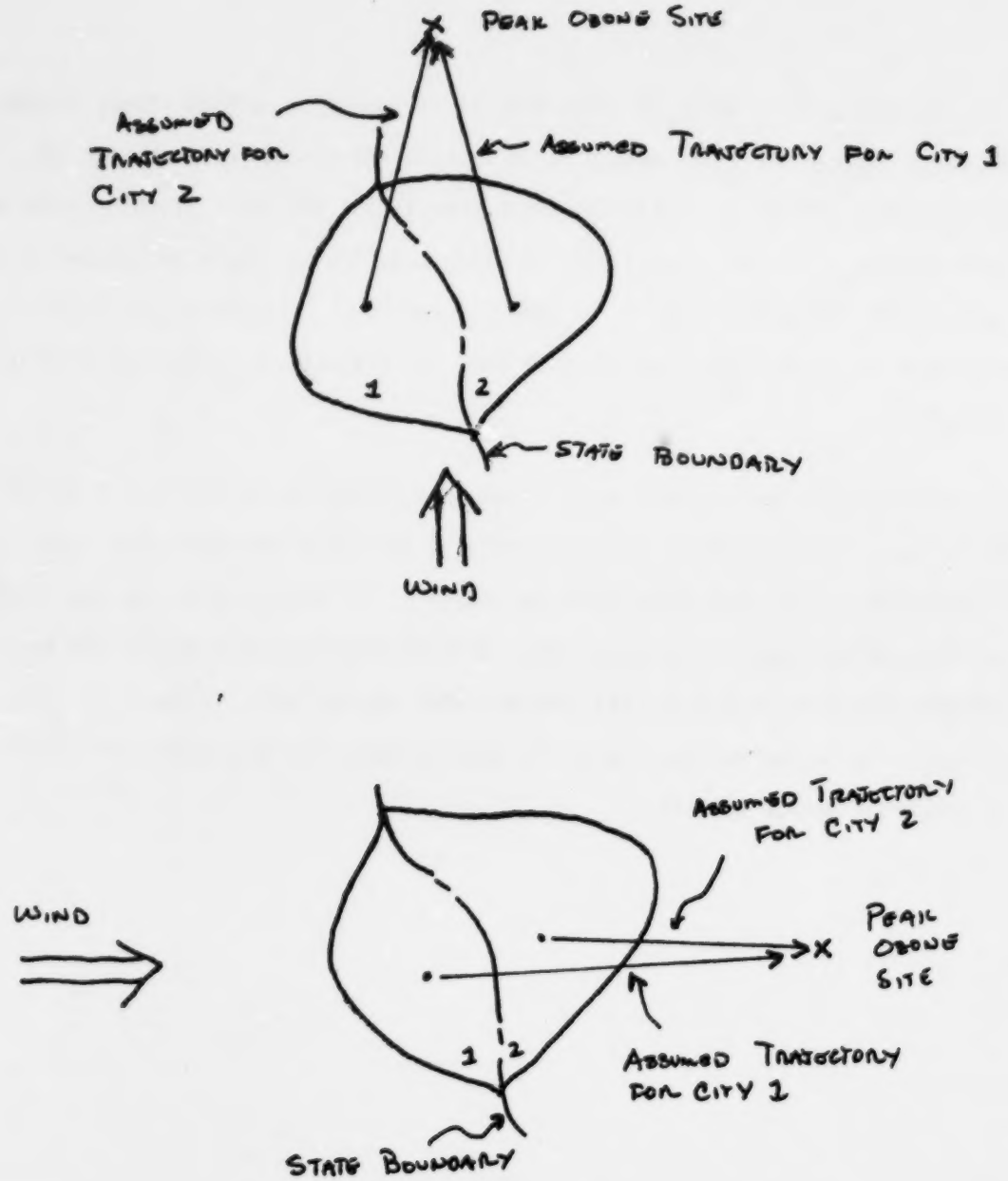

Figure B-3. Illustration of the Treatment of Contiguous Urban Areas.

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ADDENDUM TO EKMA GUIDELINE DOCUMENT
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March 1981

SECTION A.1.2 (page A-2)

The phone number for the National Climatic Center listed in the EKMA Guideline document is for users who want a whole year's radiosonde data on a computer tape. If radiosonde data for selected days are needed, they can be obtained on hard copy by calling (704) 258-2850, extension 683.

The cost for computer tapes with a year (or any part of a year) of radiosonde data from one station is as follows (each tape has one year's data for one station):

--$85 for the first tape

--$45 for each additional tape

The cost for hard copy (from the new number above) is $0.60 per sounding. At stations with the usual two soundings per day, the cost is $1.20 a day per station. Orders for hard copy must total at least $5.00.